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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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 $f(a) = 1$, $f(b) = 2$, $f(c) = 3$, $f(d) = 4$, $f(e) = 5$.

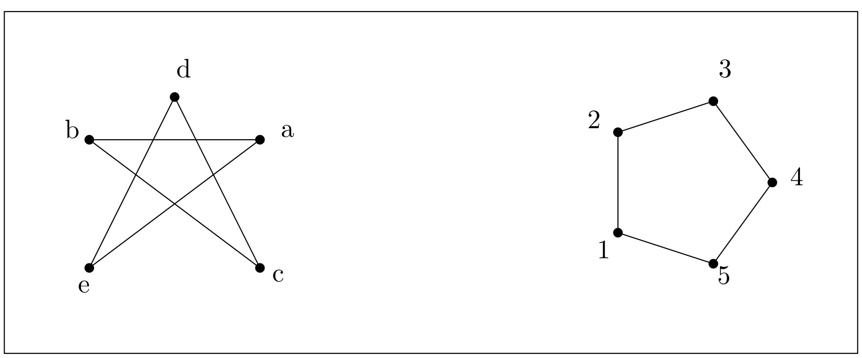

Figure 1.1: This figure depicts the graph isomorphism shown in Table (**??**) between V_1 and V_2 in the plane.

To visualize a graph, G, we create a *drawing* Γ, 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. 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 $K_{3,3}$ [**?**]. A combinatorial *embedding* is a planar drawing with a corresponding circular order of the neighbors

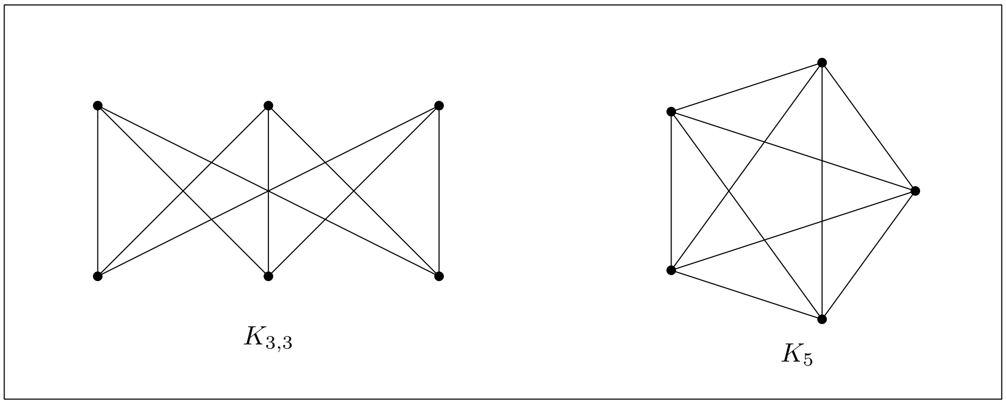

Figure 1.2: The K_5 and $K_{3,3}$ drawn in the plane.

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. In figure 1.3, the wheel graph is depcted in two different drawings, one on the left and one on the right.

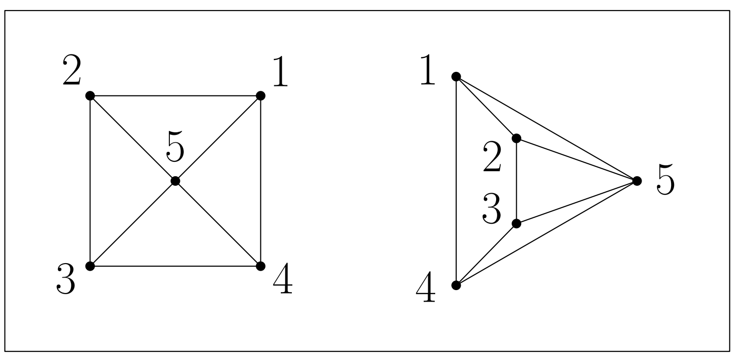

Figure 1.3: Here is a wheel graph, W_5, in two separate drawings with the same counterclockwise ordering of neighbors for each vertex.

The drawings have the followings counterclockwise order of neighbors for each vertex: Referencing table **??** and figure 1.3, we realize that the two drawings of W_5 are equivalent.

Vertex	Left Drawing	Right Drawing
1	$(2,5,4)$	$(4,2,5)$
2	$(3,5,1)$	$(1,3,5)$
3	$(2,4,5)$	$(2,4,5)$
4	$(1,5,3)$	$(1,5,3)$
5	$(2,3,4,1)$	$(1,2,3,4)$

Table 1.2: A table showing the counter clockwise circular ordering of neighbors for the left and right drawing in Figure 1.3. Note that the permutation cycles are equivalent for the right and left drawings.

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.

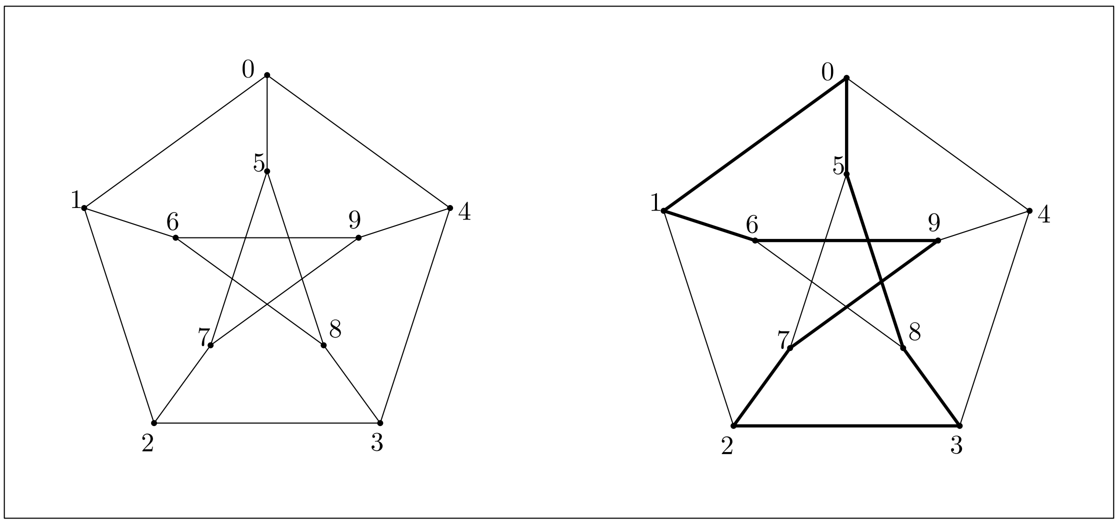

Figure 1.4: An embedding of the Peterson graph with a simple cycle of (2,7,9,6,1,0,5,8,3).

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.

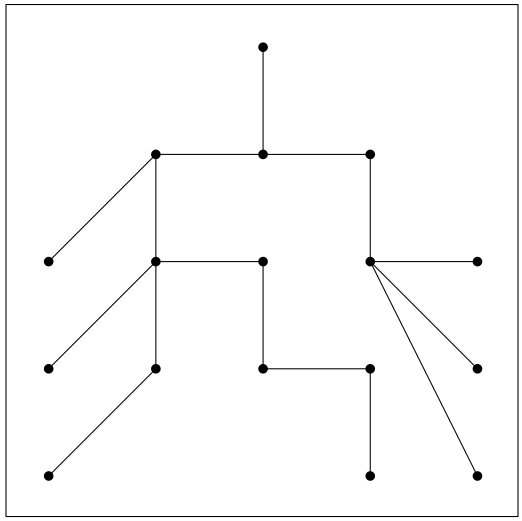

Figure 1.5: An example of a tree.

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.

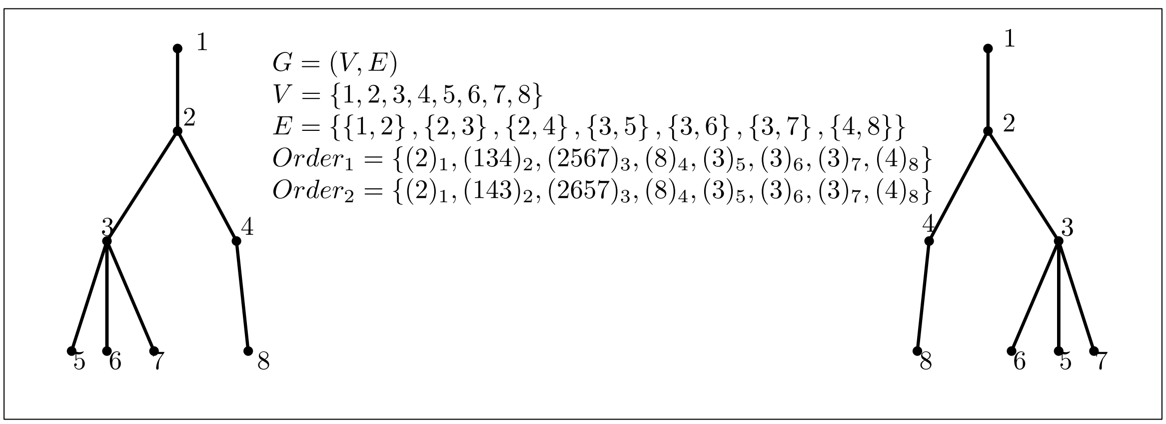

Figure 1.6: A tree with two embeddings with different cyclic orderings around vertices.

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 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

When graph drawings model physical objects, other qualities about 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

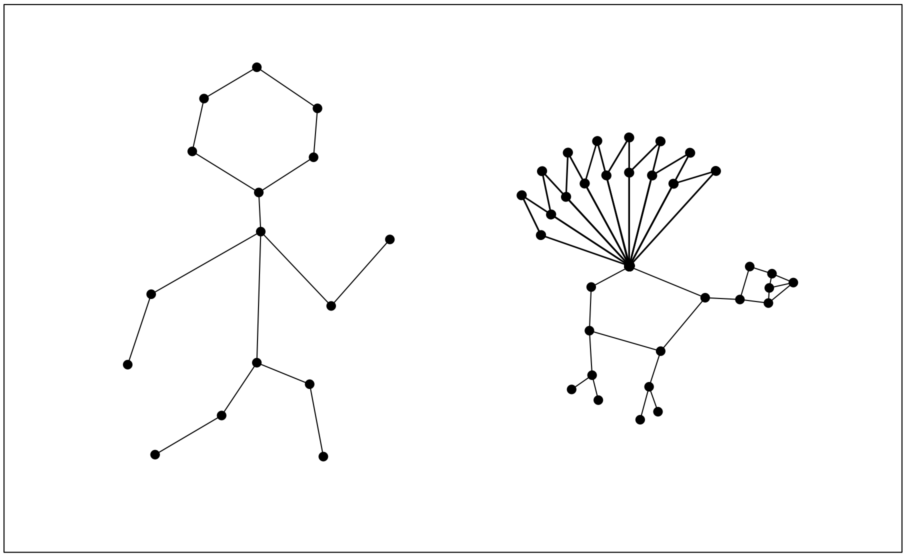

Figure 1.7: Here are skeleton drawings of a human and a turkey. When animating skeletons, one tends to make sure that the lengths of the skeleton segments are kept the same length throught the animation. Otherwise, the animation may depart from what is ideally understood of skeletal motions.

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 linkage realizations do not allow for reflection transformations.

These two types of realization types allow one to pose two different types of problems, the realizability problem for polygonal linkages and the realizability problem for polygonal linkages with fixed orientation:

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

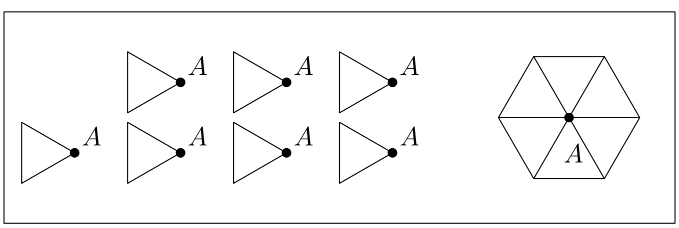

Figure 1.8: Here we have 7 congruent copies of an equilateral triangle with a hinge point of A. The polygonal linkage is not realizable. The best we can realize is at most 6 congruent copies of an equilateral triangle with the hinge point of A in the plane.

Figures 1.8 and **??** demonstrates that not all polygonal linkages have a planar realization.

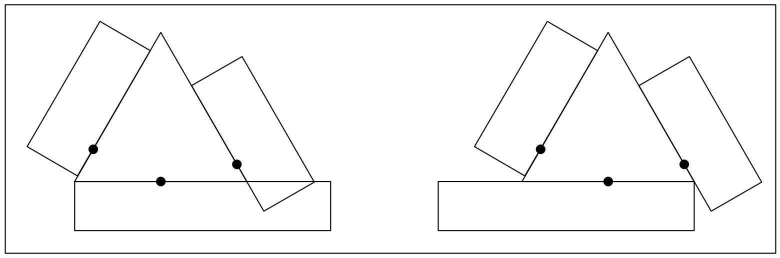

Figure 1.9: This example shows yet another example where two realizations of the same polygonal linkage. One realization where there is an intersection and another where there isn't an intersection.

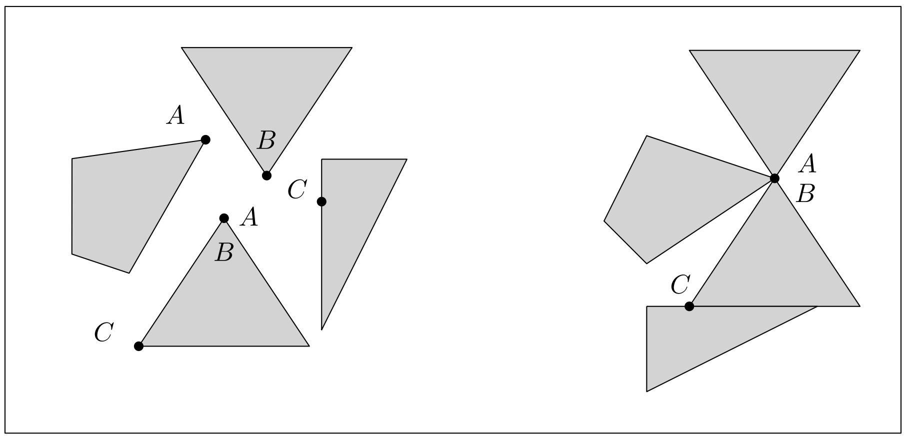

Figure 1.10: (a) A polygonal linkage with a non-convex polygon and two hinge points corresponding to three polygons. Note that hinge points correspond to two distinct polygons.(b) Illustrating that two hinge points can correspond to the same boundary point of a polygon.

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

In figure **??**, we show that orientation of polygons can alter the realization. In addition, figure **??** shows that changing the order of the polygons A, B, and C can be the difference between a realization without intersection of polygons and a realization with intersection of polygons.

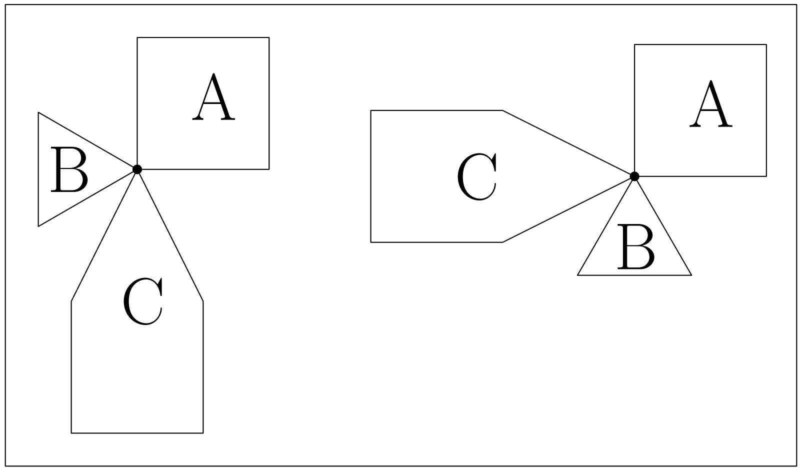

Figure 1.11: The realizations of the polygonal linkage with order (A,B,C) differs (A,C,B)

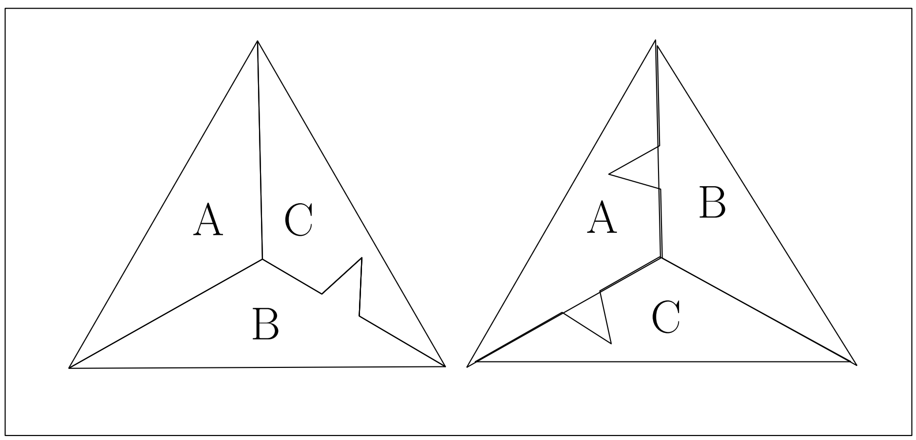

Figure 1.12: Here we have two realizations of a polygonal linkage with two different clockwise orderings (C,B,A) and (B,C,A) respectively. Note that the realization with ordering (B,C,A) has polygonal intersection.

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).

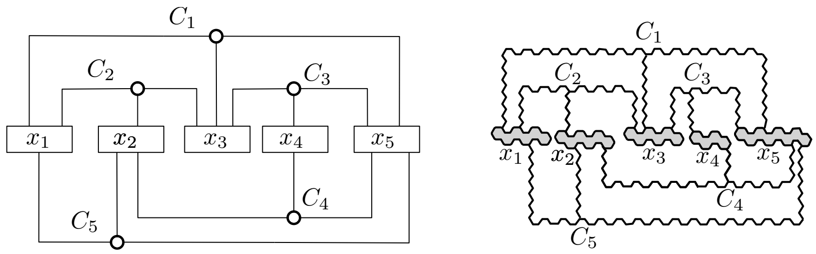

Figure 1.13: Left: the associated graph $A(\Phi)$ for a Boolean formula Φ. Right: the schematic layout of the variable, clause, and transmitter gadgets in our construction.

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.

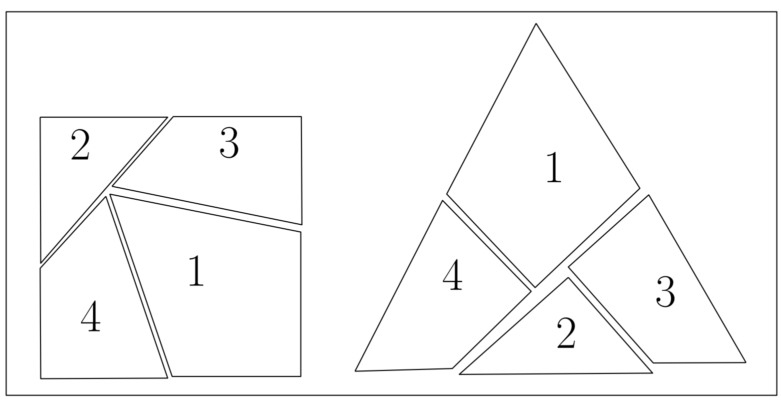

Figure 1.14: The Haberdasher problem was proposed in 1902 and solved in 1903 by Henry Dudeny. The dissection is for polygons that forms a square and equilateral traingle

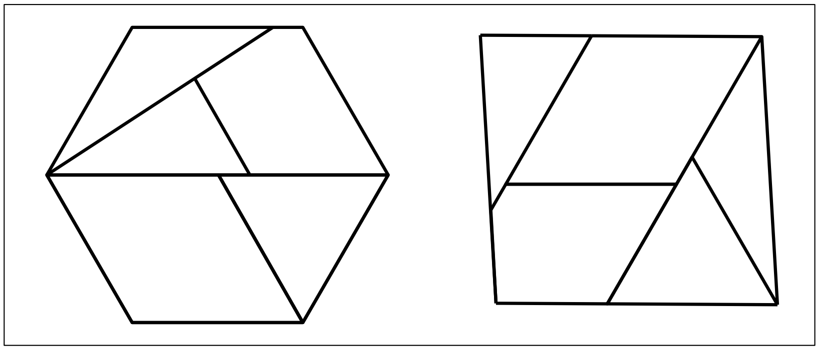

Figure 1.15: Two configurations of polygonal linkage where the polygons touch on boundary segments instead of hinges. These two realizations of the polygonal linkage are invalid to our definitions.

Geometric dissections are closely related to polygonal linkages. Figure 1.15 shows two arrangements of the same polygons to form a hexagon and a square. The reason these polygons are not polygonal linkages is that the polygons do not have consistent hinge points. Figure 1.16, shows the Haberdasher problem with hinges. This makes the Haberdasher problem as a type of polygonal linkage where the polygons are free to move about their hinge points and take the form of a triangle or square.

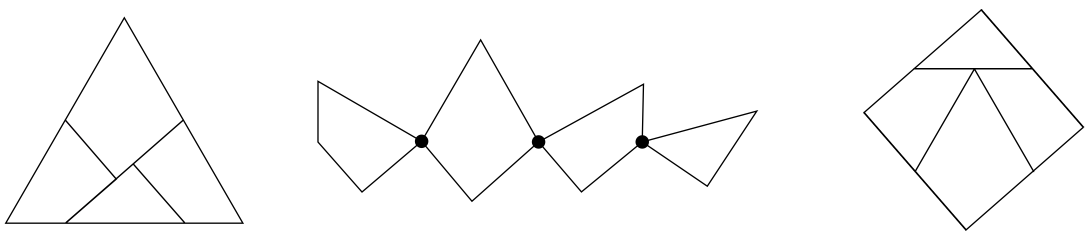

Figure 1.16: This shows the Haberdasher problem in the form of polygonal linkage.