Computational Polygonal Entanglement Theory *

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Abstract

In this paper we are concerned with motions for untangling polygonal linkages (chains, polygons and trees) in 2 and 3 dimensions. We say that an open, simple polygonal chain can be straightened if it can be continuously reconfigured to a sequence of collinear segments in such a way that the rigidity and length of each link and the simplicity of the entire chain are maintained throughout the motion. For a closed chain (simple polygon) untangling means convexification: reconfiguration to a convex polygon. For a tree untangling means "flattening". Linkages that cannot be untangled are called locked. Whether a simple open chain in 2D can be straightened remains a tantalizing open problem. For some special classes of chains it is known that they can be straightened. On the other hand a tree can lock. In 3D both open and closed chains can lock without being knotted. An open chain can be straightened if it has a simple orthogonal projection onto some plane. Furthermore, a planar closed simple chain in 3D can be convexified in a polynomial number of simple moves. A simple move is one in which only a constant number of joints can rotate at once. In this paper we review these and other recent results. In addition we describe some variants of the problem proposed by Cauchy in 1813 and Erdős in 1935.

1 Introduction

Folding and unfolding problems concerned with surfaces and linkages have received considerable attention in the computational geometry literature recently [21]. In this paper we are only concerned with "unfolding" linkages. Consider an idealized open polygonal chain linkage in the plane consisting of straight links joined together end-to-end, such as the five-bar linkage illustrated in Figure 1. We assume that the links are free to rotate about their joints in the plane but cannot cross each other at any time. In other words, the linkage must remain a simple polygonal chain during any motion. We are interested in the question of whether any simple such linkage can always be straightened. By straightened we mean that every joint has an angle of π. It is easy to see that the five-bar linkage of Figure 1 (a) can be reconfigured to that shown in Figure 1 (b) by successively straightening one end of the linkage starting at end point B. It is not so easy to answer this question for a more complicated linkage, and at this writing it remains an unsolved problem whether all such linkages can be straightened. However, Joe Mitchell has created a complicated configuration of a chain that he believes is locked. He and O'Rourke, among others, are trying to prove that it is locked [19].

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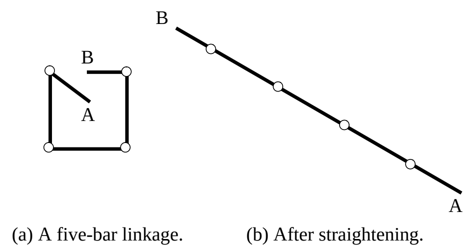

Figure 1: The simple polygonal chain in (a) can be reconfigured to that shown in (b).

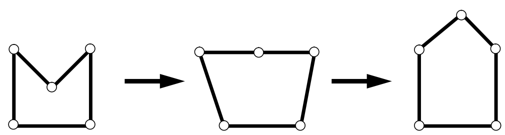

Figure 2: The closed polygonal linkage on the left can be convexified.

An analogous problem concerns planar *closed* polygonal linkages. In this case we are interested in whether a closed polygonal linkage can be *convexified*: reconfigured into a convex polygon while maintaining simplicity. For example, the concave closed five-bar polygonal linkage in Figure 2 on the left can be convexified to a pentagon by first reconfiguring the linkage into the convex quadrilateral shown in the middle figure. It also remains an open problem whether all closed linkages can be convexified. Of course if an open chain can be found that is locked a similar locked example for closed chains can be obtained by doubling all the edges. These problems have applications to robotics [16], manufacturing [2], knot theory [18] and molecular biology [13].

Before discussing some special cases of the above problems for which solutions are known, we look at some variants of these problems that have been proposed and investigated quite some time ago. One is a problem on convexifying closed simple polygons proposed by Paul Erdős in 1935 and the other is a problem of opening a convex linkage, due to Augustin Cauchy in 1813. However, to discuss the latter problem we must take a detour to Alexandria in 300 B.C. where Euclid discussed the simplest of all linkage straightening problems: his Proposition 24 in Book 1 of *The Elements*.

1.1 Euclid's Caliper Linkage

The simplest possible polygonal linkage is a two-bar linkage (also called an *elbow* [16]) with one joint that resembles a jackknife. It is obvious that such a linkage can be straightened. One merely has to rotate one segment until it is collinear with the other and the angle at the joint equals π. Therefore a more interesting problem concerning two-bar linkages is the *caliper lemma* [25]. This

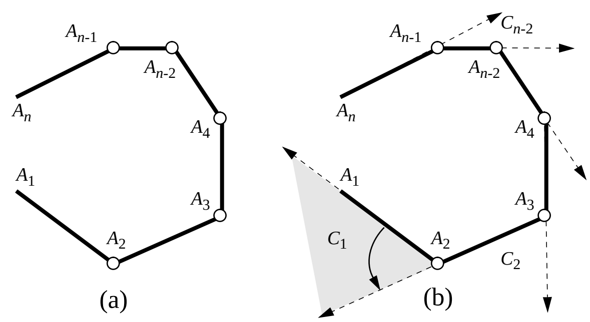

Figure 3: A linkage of n-links in convex position can be straightened.

lemma states that as you open the caliper so that the smaller angle at the joint is bigger, the ends of the caliper move a greater distance apart. This result is in essence Euclid's Proposition 24 in Book 1 of *The Elements*. Furthermore, this proposition forms one of the corner stones for many of the most recent results in this area.

1.2 Cauchy's Convex Linkage

A natural generalization of Euclid's two-bar linkage is a linkage $A = A_1A_2...A_n$ consisting of $n-1$ links in convex position such as that illustrated in Figure 3. We say that a linkage is in convex position if when we join the two ends with a line segment we obtain a convex polygon. That all such linkages can be straightened is easily established. For every link A_iA_{i+1} construct a ray starting at A_{i+1} in direction A_i, and let C_i denote the resulting cone defined by the two rays starting at A_{i+1} and A_{i+2}, respectively. Because the linkage is in convex position the cones C_i are all empty. This property suggests the following unfolding motion. Rotate A_1A_2 about A_2 so as to sweep A_1A_2 through the cone C_1 until it is collinear with A_2A_3. This motion leaves the cones $C_2, C_3, ..., C_{n-2}$ unchanged. Now we consider $A_1A_2A_3$ as one link A_1A_3 and rotate it about A_3 in cone C_2. We continue this process unhindered until the chain is collinear with A_nA_{n-1}. Therefore the straightening property of Euclid's two-bar linkage extends to the convex $(n-1)$-bar linkage.

The question now arises: does the *caliper lemma* apply to this more general situation? In other words, when the $(n-1)$-bar convex linkage opens to a new convex configuration, do the ends also move apart? The answer is *yes* and the result is known as *Cauchy's Lemma* after the French mathematician Augustin Cauchy who first investigated the problem in 1813 in the context of his famous rigidity theorem for convex polyhedra [9].

Let us examine how Cauchy [9] tried to prove the theorem. We say *tried* because, although his theorem is correct, his proof is not. We invite the reader to spot the flaw before we expose it.

Theorem 1 *(Cauchy's Lemma) If we transform a convex linkage $A = A_1A_2...A_n$ into another convex linkage $B = B_1B_2...B_n$ by opening all joints $A_2A_3...A_{n-1}$, or by opening some joints and leaving the remaining joints unchanged, then the linkage ends A_1 and A_n move apart, that is, the distance between B_1 and B_n is greater than the distance between A_1 and A_n.*

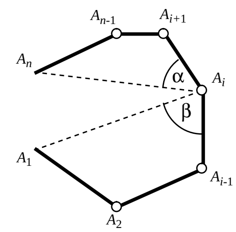

Figure 4: Illustrating Cauchy's proof when one joint is opened.

Proof: (Cauchy's incorrect "proof") For the case $n = 3$ Euclid's caliper lemma establishes the result. Therefore consider the case when n is greater than three. Let A_i be one of the k joints that opens to the angle at B_i and let us first open only this joint and leave the remaining joints unchanged (refer to Figure 4). Then the linkage $A_iA_{i+1}...A_n$ rotates rigidly in a clockwise direction about A_i. Similarly, the linkage $A_1A_2...A_i$ rotates rigidly in a counter-clockwise direction about A_i. Therefore, the angles $\alpha =$ angle $A_nA_iA_{i+1}$ and $\beta =$ angle $A_1A_iA_{i-1}$ remain fixed during the rotation. Furthermore, since angle $A_{i-1}A_iA_{i+1}$ has increased it follows that angle $A_1A_iA_n$ has increased. Finally, since the distances $d(A_n, A_i)$ and $d(A_1, A_i)$ remain fixed during the rotation we conclude by applying Euclid's caliper lemma to the "caliper" $A_1A_iA_n$ that A_1 and A_n have moved apart.

If more than one joint of A is opened we consider one joint at a time and proceed as above until all k joints have been opened. Since at each such opening the distance between A_1 and A_n increases it follows that when we are finished $d(B_1, B_n) > d(A_1, A_n)$. ■

Although not explicitly stated, Cauchy is attempting a proof by induction on the number of joints opened. Let us assume that k joints are to be opened. First we establish the *base case*: $k = 1$. We need to show that when one convex linkage $A_1A_2...A_n$ is transformed into another convex linkage $B_1B_2...B_n$ by opening *one* joint A_i then the ends A_1 and A_n move apart. Up to this point Cauchy's proof is not only correct, but executed in a most elegant manner by converting the problem to Euclid's caliper lemma. Now when $k > 1$ we assume the result holds when we open $k - 1$ joints (the *induction hypothesis*) and must prove it is true when we open the k joints. After proving the base case $k = 1$, Cauchy describes a procedure for opening all k joints by considering one joint at a time. The implicit reasoning here is that once we have opened one of the k joints we obtain a linkage in which we must open only $k - 1$ joints for which we invoke the induction hypothesis. Not only does Cauchy not state the induction hypothesis, but he does not prove that his method works. Furthermore, it fails precisely because the induction hypothesis breaks down.

Consider the three-bar linkage $A_1A_2A_3A_4$ in Figure 5 (a). We would like to open the $k = 2$ joints A_2 and A_3 so that the angles at B_2 and B_3 are right angles. In this way we satisfy the input-output conditions of the problem that linkages $A_1A_2A_3A_4$ and $B_1B_2B_3B_4$ are both convex. Following Cauchy's procedure we first open one joint A_2 as in Figure 5 (a). Now we have a linkage in which only $k - 1$ links are to be opened and would like to invoke the induction hypothesis to finish the proof. But the induction hypothesis specifies that the linkage must be *convex* and this is clearly not the case since A_4 lies in the interior of triangle $B_1A_2A_3$.

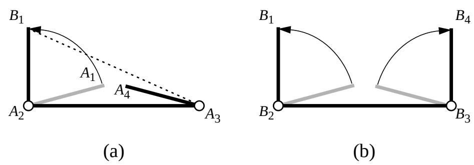

Figure 5: A counter-example to Cauchy's proof.

Furthermore, for non-convex linkages the theorem is false. For example, consider again the linkage $B_1A_2A_3A_4$ in Figure 5 (a). If we open joint A_3 so that A_4 moves to A_4' and such that angle $A_2A_3A_4'$ < angle $A_2A_3B_1$ + angle $A_4A_3B_1$, then B_1 and A_4 actually move closer together and $d(B_1, A_4') < d(B_1, A_4)$. This flaw in Cauchy's proof went unnoticed for over 120 years until Ernst Steinitz uncovered it and together with Rademacher provided a correct but very long and complicated induction proof [26]. A similar long proof is described by Lyusternik [17]. Since then many other proofs of Cauchy's arm lemma, as it is also called, have appeared. The shortest and most elegant induction proof is due to S. K. Zaremba [24]. It is so beautiful in fact that it was chosen to appear in *Proofs from THE BOOK* by Martin Aigner and Günter M. Ziegler [1]. This book, dedicated to the memory of Paul Erdős, contains a selection of the most beautiful proofs, brilliant ideas, clever insights, wonderful observations and tantalizing open problems in the world of mathematics.

2 Open Chains

In the previous section we concentrated on the problem of opening planar convex polygonal linkages by increasing both the interior angles of the joints and the distance between the endpoints of the linkage. Here we return to the original problem of actually straightening the linkages. As pointed out earlier, no one has yet proved or disproved whether every linkage can be straightened. On the other hand, as Figure 3 illustrates, straightening convex linkages is trivially accomplished by straightening one joint at a time, in order, starting from either endpoint. Furthermore, it is clear that the procedure works also for some non-convex linkages such as the *spiral* linkage in Figure 1 (a) as long as one starts the unfolding from the *outer* endpoint of the linkage. Therefore it is only natural to ask how powerful this simple-minded *jackknife* motion is for straightening more general classes of linkages. Several more general classes of polygons have been investigated in [6] where jacknife motions and other simple motions in which only two joints rotate simultaneously are allowed. In particular, [6] contains $O(n)$ time algorithms that use $O(n)$ simple motions to straighten *hull-expanding* and *doubly-visible* chains and an $O(n \log n)$ time algorithm for $O(n)$ simple motions to straighten *same-side-visible* chains. A chain is hull-expanding if, as we compute the convex hull of the chain starting at one end, the next link always lies outside the convex hull of the links examined so far. Here jackknife motions suffice. A chain is doubly-visible if for each point on the chain there exists a line that intersects the chain only at this point. Finally, a chain is same-side-visible provided there exists a line such that the chain is to one side of the line and for each point on the chain there exists a ray on the same side of the chain that intersects the chain only at that point and also intersects the line.

Arkin et al., [2] call jacknife motions from one end "all-or-nothing" straightening and solve several foldability problems for chains (by applying the straightening in reverse order) under various manufacturing constraints. They also prove that certain problems of determining if planar linkages can be straightened are hard.

In 3D it is shown in [3] that a chain which admits a simple projection onto some plane can be straightened with $O(n)$ simple motions.

3 Polygons

Not much is known concerning which classes of polygons in 2D can always be convexified. Everett et al., [12] show that star-shaped polygons can be convexified in $O(n^2)$ time using $O(n)$ complex motions. Each such motion is a radial expansion and rotates $O(n)$ joints simultaneously. Biedl et al., [5] prove that a monotone polygon can be convexified in $O(n^2)$ time using $O(n^2)$ simple motions, where each such motion rotates no more than four joints simultaneously. It is conjectured that equilateral polygons can always be convexified.

3.1 Erdős Flips

Before discussing how linkages in three dimensions might be untangled, if at all, we consider a convexification problem which could be considered to be in between two and three dimensions. Let $A = A_1A_2A_3A_4$ be a closed non-convex four-bar linkage in the two-dimensional xy-plane with A_3 as its reflex joint. Assume that $A_1A_4 = A_1A_2$ and $A_2A_3 = A_3A_4$. Furthermore, assume that the linkage (although planar) is embedded in the 3D space with axes x, y and z, that the joints are *ball-joints* which allow rotations in all directions in 3D and that, as usual, no two links may cross during any motion. If we lift joint A_3 off the xy-plane into the third dimension z (leaving the other three joints fixed) by rotating it about the line through A_2 and A_4 until it returns to the xy-plane at position B_3, then the linkage has been convexified with one simple motion. This rotation motion in 3D is equivalent to a reflection transformation in the xy-plane: B_3 is the reflection of A_3 across the line through A_2 and A_4.

A natural more general question is: given any planar closed linkage in 3D, can the third dimension be helpful, with motions similar to those described above, for convexification? This problem has been discovered and re-discovered independently by several mathematicians, and more recently, computer scientists dating back to 1935, the latter group motivated by practical robotics problems with linkages, and the former by simple curiosity about the geometric properties of polygons and simple closed curves [23], as well as the computer exploration of knot spaces [18] .

The first person to propose this problem was Paul Erdős in 1935 [11] in the context of planar polygons. Consider the linkage as the boundary of the simple polygon P in Figure 6 (a). If we subtract this polygon from its convex hull we obtain the convex deficiency: a collection of connected regions. Each such region together with its boundary is itself a polygon, often called a *pocket* of P. The polygon P in Figure 6 (a) has two pockets P_1 and P_2. Each pocket has an edge which coincides with a convex hull edge of P (shown in the figure by dotted lines). Such an edge is called the pocket *lid*. Erdős defined a reflection operation on P as a simultaneous reflection of all the pockets of P about their corresponding pocket lids. Applying a reflection operation to polygon P in Figure 6 (a) yields the new polygon P' in Figure 6 (b). In 1935 Erdős conjectured that given any simple polygon, a *finite* number of such reflection operations will convexify it. The first proof of Erdős' conjecture was provided in 1939 by Béla Nagy [20]. First Nagy observed that reflecting *all* the pockets in one step can lead from a simple polygon to a non-simple one. Therefore he modified

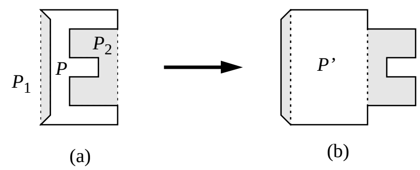

Figure 6: Flipping the pockets of a polygon.

Erdős' problem slightly by defining one step to be the reflection of only *one* pocket. Since a pocket is reflected into a previously empty half-plane (because a pocket lid is a line of support of P) no collisions can occur with such a motion. Let us call such an operation a *flip*. Nagy then proceeded to prove that any linkage (simple polygon) can be convexified by a *finite* number of flips. Since 1939 there have been many rediscoveries of this problem, surprisingly, no author aware of the results of the other authors. The latest rediscovery was in 1998 by Biedl et al., [3], and Grünbaum [14] has given an account of some of these. I have since discovered additional instances and a survey of these papers along with a simplified elementary proof of the Erdős-Nagy theorem that borrows the best from the existing proofs is forthcoming [28].

Although the Erdős flips will convexify any simple polygon in a *finite* number of steps, this number cannot be bounded as a function of n. Given any positive integer k it is possible to construct a polygon (indeed a quadrilateral) that will need at least k flips [3], [14]. On the other hand, Biedl, et al. [3] have shown that with the *line-tracking* motions of Lenhart and Whitesides [16] any planar simple polygon in 3D can be convexified in $O(n^2)$ time with $O(n^2)$ simple motions.

3.2 Locked Unknotted Polygons in 3D

The space of closed chains or polygons of n line segments with lengths $l_1, ..., l_n$ embedded in R^3 as unknots (also trivial knots) is denoted (using the notation of Cantarella and Johnston [8]) by $Pol_n(l_1, ..., l_n)$. In 1998 Cantarella and Johnston [8] and independently, Biedl, et al. [3] studied the embedding classes of such objects and discovered that there exist stuck (or locked) simple polygons. The polygon of Biedl, et al. [3] contains 10 edges whereas the example of Cantarella and Johnston [8] has only six edges (see Figure 7). These results are relevant to linkage convexification problems because they imply there exist simple linkages in 3D that cannot be convexified. The results are also relevant to understanding how small-scale rigidity influences the shape of DNA and other complex molecules [15]. Since, in addition to the flat convex version, there are "right" and "left" handed versions of the unknot in Figure 7 , Cantarella and Johnston in effect proved that the space of isotopic embeddings of the hexagon has at least three connected components. The lengths of the edges are crucial for this property. Indeed, if all six lengths are the same, Millet and Orellana [18] showed that the class of unknots in $Pol_6(1,1,1,1,1,1)$ is connected. Furthermore, if we consider orientation Calvo [7] has shown that there are distinct embeddings of left and right-handed trefoils in $Pol_6(1,1,1,1,1,1)$. Cantarella and Johnston conclude that they suspect that all stuck unknots in Pol_6 belong to the class illustrated in Figure 7, in other words, that there are no more than three components in Pol_6. However, recently I discovered a new class of stuck unknotted hexagons [27]. An example of a hexagon in this new class is shown in Figure 8.

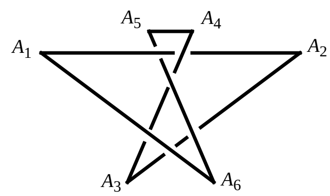

Figure 7: The stuck unknot in Cantarella and Johnston [8].

Denote the space polygon by its vertices $A = A_1A_2...A_6$ and let l_i be the length of link A_iA_{i+1}, modulo 6. Note that the lengths in both figures are not metrically accurate but the figures are easier to visualize as shown. Intuitively the only way to convexify the polygon with the knot diagram shown is to either pass the chain $A_3A_4A_5A_6$ over A_1 or under A_2. For this to occur it is necessary that the length of $A_3A_4A_5A_6$ be not smaller than the length of the shorter of l_2 and l_6 . However, it is possible to construct such hexagons that violate these distance requirements. For example, a polygon with the knot diagram shown in Figure 8 is stuck if it has the following coordinates. $A_1 = (100, 10, 0), A_2 = (-100, 10, -1), A_3 = (10, 20, 0), A_4 = (10, 0, 10), A_5 = (-10, 0, -10), A_6 = (-10, 20, 0)$.

Furthermore, the hexagon in Figure 8 is in a sense more stuck than the hexagon in Figure 7. Let us define the *stuck number* of a polygon as the minimum number of links that must be removed so that the remaining open chains can be straightened. Then, if the stuck number of a polygon is k we will say the polygon is k-stuck. Let us call a polygon *weakly* k-stuck if the removal of *any* k links allows the remaining open chains to be straightened. Similarly, let us call a polygon *strongly* k-stuck if this is not the case but there exists *some* set of k links whose removal allows subsequent straightening. Using the results of Cantarella and Johnston [8] it can be shown that the hexagon in Figure 7 is *weakly* 1-stuck whereas the example in Figure 8 is *strongly* 1-stuck. Indeed, if in the hexagon of Figure 8 the link A_1A_2 is removed we obtain the stuck *knitting-needles* example of Cantarella and Johnston [8] and Biedl et al. [3].

It is clear from the example in Figure 8 that here we also have left and right handed versions of the polygon. Therefore we have the following result.

Theorem 2 *(Toussaint [27]) For suitable choices of edge-length, there are at least five classes of embeddings of the unknot in Pol_6*

We note that just as in the example of Cantarella and Johnston, we can obtain a family of stuck unknots similar to the polygon in Figure 8 for any value of $n > 6$ by inserting a polygonal chain of any number of edges between A_4 and A_5 as long as their total length does not exceed the length l_4. As a final remark we add that although hexagons in 3D can be knotted, any simple polygon with less than six edges is unknotted [22].

In contrast to the result in 3D, recently Cocan and O'Rourke [10] have shown that for all dimensions greater than 3 every simple open chain may be straightened, and every simple closed chain may be convexified. The algorithms run in polynomial time.

We close this section by mentioning a couple of additional open problems. (1) A natural generalization of convexifying a planar polygon in 3D is to consider more general polygons that admit a simple projection onto some plane. It is conjectured that all such polygons can be convexified.

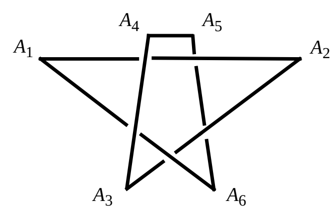

Figure 8: A new class of stuck unknotted hexagons (Toussaint [27]).

(2) Since I discovered the stuck unknots of Figure 8 I have heard from Heather Johnston and Jason Cantarella that they, together with Jouko Koskinen have also just discovered this class. The conjecture now is that there are no more than five classes of non-trivial embeddings of hexagons in 3D.

4 Tree Linkages

A *tree linkage* is a linkage that has the form of a tree. As before, nodes are joints that can rotate and the edges are links that remain rigid in the sense that they do not bend and their length is preserved during any motion. The *tree linkage reconfiguration* problem is: given two configurations, can one be moved to the other. The *flattening* problem can be described as follows. Hang the tree linkage from any joint acting as the root so that the children of every joint are pointing downward and the aspect ratio of the linkage is as large as desired without allowing any links to cross during the motion. Biedl et al. [4] show that not every tree linkage can be straightened.

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