Fixed-Angle Polygonal Chains: Locked Chains and the Maximum Span

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Contents

[1] These definitions are based on those in [DO06] and [DLO05]

[2] This section was first drafted by Joseph O'Rourke to provide motivation for our study of maxspans.

[3] From this section onward, the results reported were obtained in direct collaboration with Joseph O'Rourke.

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Acknowledgements

This research was done in conjunction with Joseph O'Rourke, my thesis advisor. Thanks also to my readers, Mike Albertson and Chris Golé, as well as the Smith College math department.

1 Introduction

This thesis investigates two properties of fixed-angle polygonal chains: (1) conditions for locking near-unit chains, and bounds on length ratios when the precise conditions seem inaccessible; (2) the *maximum span* of a fixed-angle chain, that is, the largest distance achievable between its endpoints.

1.1 Basic Definitions [4]

A *polygonal chain*, or just a *chain*, is a non-self-intersecting sequence of line segments (in 2D or 3D) connected end-to-end. The *edges* are also called *links*, and the *vertices* are also called *joints*. The *joint angle* at a vertex v_k refers to the angle between the edges $v_{k-1}v_k$ and v_kv_{k+1}. If there is no constraint on the joint angles, the chain has *universal joints*. A *fixed-angle chain* is one in which each joint angle at each vertex is some fixed angle α_i. If all joint angles of the chain are fixed to the same angle α, it is called an α-chain. These α-chains are our main (although not sole) focus. We will occasionally refer to the *turn angle* τ rather than the joint angle α, which is defined to be $\tau = \pi - \alpha$.

A chain is *locked* if its configuration space has two or more connected components. This means it cannot be reconfigured between some pair of distinct embeddings without self-intersection. A chain all of whose link lengths are equal is an *equilateral chain*. Because we take this fixed length to be 1, we also use the term *unit chain*. The *length ratio* L of a chain is the ratio of the longest link length to the shortest link length. The standard 5-link "knitting needles" chain (with universal joints) is locked for all $L > 3$. See Fig. 19.

A chain C is called a *near-unit* chain if, for any given $\epsilon > 0$, there is a chain C' of similar relevant properties (for us: whether or not it is locked) with length ratio within $1 \pm \epsilon$. Similarly, a chain C is called a *near-α* chain if, for any given $\delta > 0$, there is an α'-chain of similar relevant properties with α' within $\alpha \pm \delta$.

[4] These definitions are based on those in [DO06] and [DLO05]

1.2 Locked Chains

The first part of this thesis concentrates on the locking of *near-unit* α-chains. Such chains have been used to model the geometry of protein backbones (which have joint angles of $\sim 109°$ and links of roughly constant length) [ST00] [DLO05]. Understanding the locking of these chains is believed to be central to predicting the native state of a protein, and furthermore, may clarify the space of possible protein foldings [DLO05]. A promising application that could stem from understanding the conditions for locking is protein folding algorithms. The configuration space being searched by current folding algorithms is vast, and may consist of predominantly locked configurations. Yet the process by which proteins fold as they emerge from the ribosome does not permit locked configurations, so removing these configurations from the searchable configuration space would increase the efficiency of folding algorithms. Hence one of our primary motivations is the pursuit of this question:

Question. Does there exist a near-unit, near-α locked chain?

We show that there is a near-unit, near-$60°$ locked 4-chain. However these bond angles of $60°$ are far from the bond angles of proteins, which are close to $109°$. Although we worked on trying to establish whether or not there are near-unit, near-α chains for bond angles closer to those in proteins—especially $\alpha = 90°$, we were unable to settle those questions. Therefore we sought the smallest *length ratio*, the ratio of the longest to the shortest link lengths, that permits locking. This led to our second main focus.

1.3 Maximum Span

The second part of the thesis concentrates on the *maximum span* of fixed-angle, polygonal chains. This latter investigation is weakly connected to lockability, in that the maximum span of a near-unit, α-chain provides a (weak) bound on the length ratio for which a locked chain exists. This was our original motivation for exploring the span of polygonal chains. However our line of investigation shifted from lockability to maximum span, an interesting problem in its own right.

As previously mentioned, fixed-angled chains can model protein backbones. Soss studied the *span* of such chains: the endpoint-to-endpoint distance. He proved that finding the minimum and the maximum span of planar configurations of the chain–the min and max *flat span*– are NP-hard problems [Sos01]. Protein backbones are rarely planar, so the real interest lies in 3D. Soss provided an example of a 4-chain whose max span in 3D is not achieved by a planar configuration, establishing that 3D does not reduce to 2D. He designed an approximation algorithm, but left open the computational complexity of finding 3D spans.

Soss concentrated on the more interesting max-span problem, and we do the same. We make progress on the 3D max-span problem by focussing on restricted classes of chains, which are incidentally among the most relevant under the protein model.

We show that the 3D max span of a unit α-chain is achieved in a planar configuration, what we call the *trans-configuration*: a flat configuration in which the joint turns alternate between $+\tau$ and $-\tau$. (The terminology is from molecular biology, which distinguishes between the trans- and cis-configurations of molecules.) We provide examples that show that, without the equal-length assumption, or without the equal-angle assumption, the max-span configuration might be nonplanar. For $90°$-chains, the max flat span is achieved by the trans-configuration, and can be found efficiently, in contrast to the arbitrary-α situation. Finally, we establish a structural theorem that permits the 3D max span of $90°$-chains to be found via a dynamic programming algorithm in $O(n^3)$ time.

Although in this thesis, I only prove the above results for $90°$-chains, we are confident that the results hold for α-chains for abitrary α, and hope to write a paper for publication with those results.

2 Near Unit, Near Fixed-Angle 4-Chains

In this section, we examine the conditions for locking near-unit, near-α 4-chains, and prove the existence of a locked 4-chain for $\alpha \leq 60$. Recall that a chain is *locked* if its configuration space has two or more connected components. This means it cannot be reconfigured between some pair of distinct embeddings without self-intersection.

Theorem 2.1 *For any $\epsilon > 0$ and any $\delta > 0$, there is a near-unit, near $60°$ locked 4-chain, that is, one with all lengths within $1 \pm \epsilon$ and all angles within $60° \pm \delta$.*

Proof: Consider the following symmetric configuration (shown in Fig. 1) of a 4-chain with vertices (a', a, o, b, b') and edges connecting adjacent vertices of the 5-tuple: Let a and b be fixed at $(-\frac{1}{2}, 0, 0)$ and $(\frac{1}{2}, 0, 0)$, respectively. Let o be fixed at $(0, \frac{\sqrt{3}}{2}, 0)$. Note that ao and ob have unit length. Select coordinates for a' such that:

$$\begin{aligned} &(1)\ aa' \text{ lies between } ob \text{ and } bb', \\ &(2)\ |aa'| = 1 + \epsilon, \\ &(3)\ (a' - a) \cdot (o - a) = (1 + \epsilon) \cos(\frac{\pi}{3} - \delta). \end{aligned}$$

Similarly choose coordinates for b' such that bb' lies above (with respect to z) aa', has length $1 + \epsilon$ and makes an angle of $\frac{\pi}{3} - \delta$ with ob. Let cone A be the cone swept out by aa' while maintaining $\angle oaa' = \frac{\pi}{3} - \delta$. Let cone B be defined analogously. If aa' lies between ob and bb' for any position of b' on cone B and a' on cone A, we say that aa' is *captured*. That is, the motion of aa' about ao is restricted to angles between bb' and ob. Refer to Fig. 2.

Our goal is to show aa' is captured between ob and bb', and that as ϵ goes to zero, so does δ, which permit us to satisfy any given (ϵ, δ) pair.

Rotate aa' such that it just touches from above ob and rotate bb' such that it just touches from above aa', so that aa' and bb' are infinitesimally close to the xy-plane; see Fig. 3. Then the equations of the lines containing aa' and bb' are $y = (x + \frac{1}{2}) \tan \delta$ and $y = (x - \frac{1}{2}) \tan(\frac{\pi}{3} + \delta)$, respectively. Solving for the intersection of aa' and bb', we obtain

$$x_{int} = -\frac{\tan \delta + \tan(\frac{\pi}{3} - \delta)}{\tan \delta - \tan(\frac{\pi}{3} - \delta)},$$

where x_{int} is the x-coordinate of their intersection point. Hence we have

$$(1 + \epsilon)^2 = (\frac{1}{2} + x_{int})^2 + ((x_{int} + \frac{1}{2}) \tan \delta)^2.$$

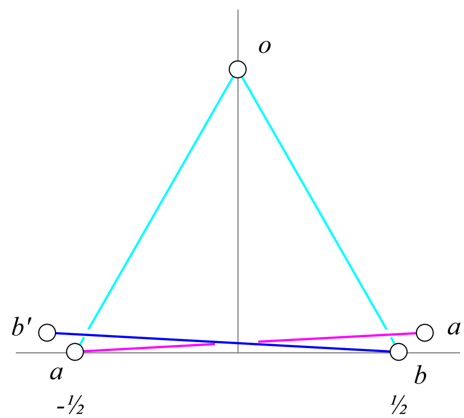


Figure 1: Configuration of 4-chain. Notice that aa' is captured between ob and bb'.

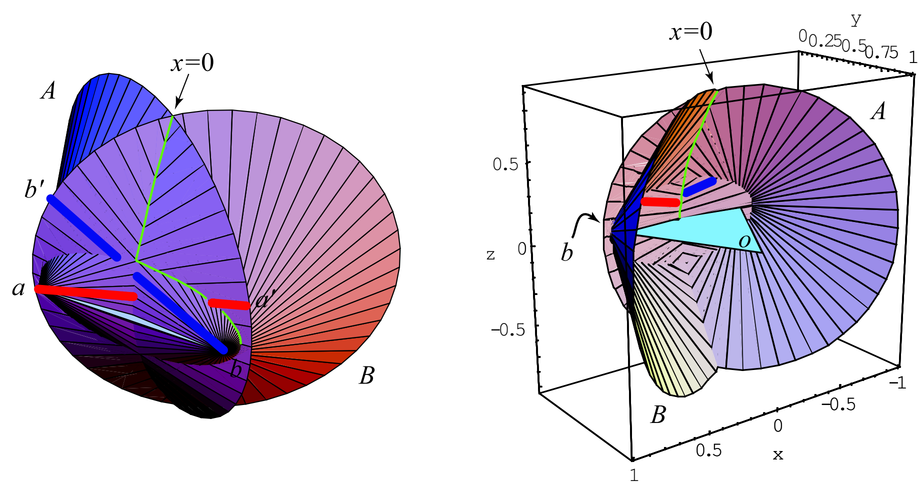


Figure 2: aa' is captured between ob and bb' inside cone B. aa' cannot reach the midplane without passing through bb' at some point along the trajectory.

The above equation allows us to write δ has a function of ϵ. Geometrically it is clear that, $\lim_{\epsilon \to 0} \delta(\epsilon) = 0$. See Fig. 3. Algebraically, as $\epsilon \to 0$ the LHS goes to 1, the RHS must also go to one, which can only happen if the second term $((x_{int} + \frac{1}{2}) \tan \delta)^2$ goes to 0, since the first term goes to 1. And the second term will only go to 0 if δ goes to 0.

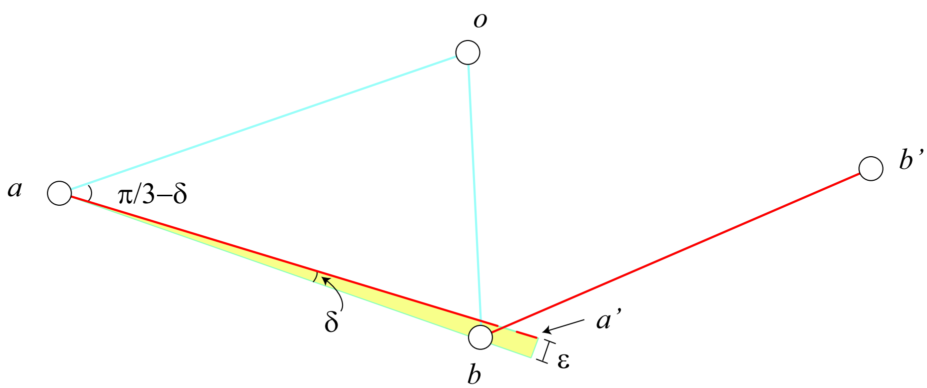


Figure 3: Geometric relationship between ϵ and δ.

Now we show that aa' is captured between ob and bb'. We will do this by showing that the conditions for escape cannot be satisfied without aa' passing through bb'. The minimum requirement for escape is that a' lies along bb' (that is, aa' just brushes by bb'). Let A be the unit vector along aa'. Then we obtain the following equations:

$$A \cdot (o - a) = \cos(\frac{\pi}{3} - \delta)$$
$$A \cdot A = 1$$
$$(a' - b) \cdot (o - b) = |a' - b| \cos(\frac{\pi}{3} - \delta)$$

where $a' = a + (1 + \epsilon)A$. A tedious calculation shows that the only solution (for appropriate ϵ and δ) is when $a' = b'$ on midplane $x = 0$. See Fig. 2. But aa' cannot reach the midplane without passing through bb' at some point along the trajectory. See again Fig. 2.

Notice that this theorem is tight in that if $\alpha > \pi/3$ there are no locked near-unit 4-chains. See Theorem 2.3. $\square$

Corollary 2.2 *For any $n \geq 4$ and $\alpha < 60°$, there exists a locked near-unit and near-α n-chain, i.e., one with all lengths within $1 \pm \epsilon$ and all angles within $\alpha \pm \delta$.*

Proof: First notice that the construction of **??** works for any $\alpha < \pi/3$, becoming easier for smaller angles to lock the chain. Now take a locked near-unit, near-α 4-chain, and simply add as many links as you like to the endpoints to obtain an arbitrarily long locked near-unit, near-α chain. □

Theorem 2.3 *There are no locked near-unit and near-α 4-chains for $\alpha > 60°$.*

Proof: Let K be a near-unit 4-chain with $\alpha > 60°$. Label vertices in the order (a', a, o, b, b') as before. Without a loss of generality, take a, o, and b to lie in the xy-plane and o and b to have coordinates $(0,0,0)$ and $(1,0,0)$, respectively. Because angle boa is greater than $60°$, the projection of a' onto the xy-plane must lie to the left of ob. (Note that if α were exactly $60°$, a' could lie directly

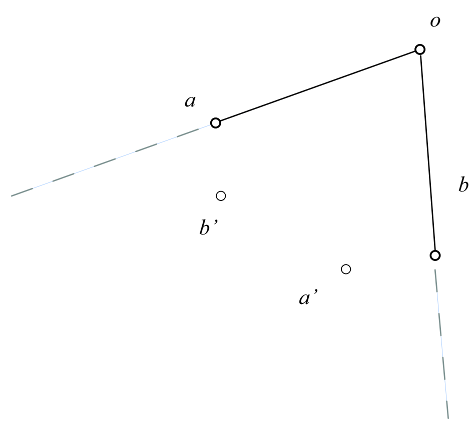


Figure 4:

on top of b and close the equilateral triangle aob.) Similarly the projection of b' must lie to the right of oa. If a' is to the left of oa or b' is to the right of ob we are done. Hence take a' and b' to lie within the angle boa. See Fig. 4. One of the edges bb' or aa' must be on top. If bb' is above aa', simply rotate bb' onto the right side of ob, such that the end links aa' and bb' lie on opposite sides of ob and hence cannot possibly intersect. If aa' is above bb', rotate aa' onto the left side of oa away from b'. This exhausts all possibilities. □

These are the first results on near-unit, near-α chains, and, unfortunately, none others are known at this time. It seems that larger α angles would lead to larger length ratios.

3 Fixed-Angle 5-Chains

By an extension of the same argument, we can prove a bound on L for 5-chains. As the reasoning is similar to that in the previous section, we only sketch the proof.

Theorem 3.1 *For any $\alpha < 90°$, there is a near-L, near-α locked 5-chain, with $L = 1/\cos\alpha$.*

Proof: *(Sketch.)* We fix v_1v_2 and v_3v_4 to have unit length. Referring to Fig. 5,

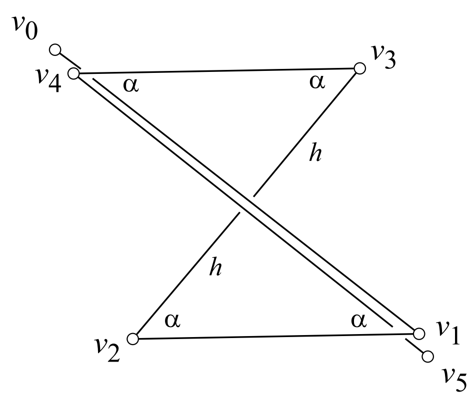


Figure 5: Taking $|v_0v_1|$ and $|v_4v_5|$ to be greater than $\frac{1}{cos\alpha}$ ensures that we can lock the chain.

taking $|v_0v_1|$ and $|v_4v_5|$ to be greater than $|v_2v_3|$ prevents the two end links from escaping, and hence, locks the chain for reasons similar to those detailed in Theorem 2.1. (In this sketch we do not repeat the reasoning.) Now we express $|v_2v_3|$ has a function of α. We have

$$h = \frac{1}{2} \cdot \frac{1}{\cos\ \alpha}$$
$$|v_2v_3| = 2h = \frac{1}{\cos\ \alpha}$$

Since making $|v_0 v_1|$ and $|v_4 v_5|$ greater than $\frac{1}{\cos\,\alpha}$ locks the chain, this gives us a length ratio $L = \frac{1}{\cos\,\alpha}$. □

This result is weak: for $\alpha = 60°$, it leads to $L = 2$ when we know 1 is achievable; for $\alpha = 70°$, it leads to $L \approx 2.9$; and $L \to \infty$ as $\alpha \to 90°$.

4 Fixed-Angle 6-chains

Stefan Langerman and Joseph O'Rourke proved that there is a near-unit, 90°, locked 6-chain for any $L > \sqrt{2}$ [LO04]. See Figs. 6 and 7.

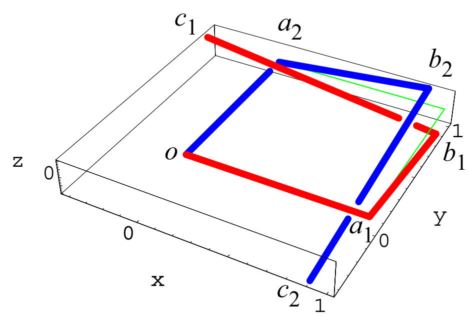


Figure 6: A near-90° locked chain with L near $\sqrt{2}$ [LO04].

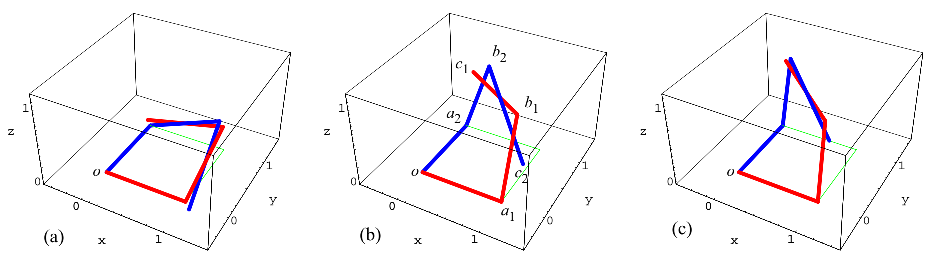


Figure 7: Animation of opening motion [LO04]. The two end links have length $\sqrt{2} + \epsilon$.

5 Planar Maximum Span Configurations

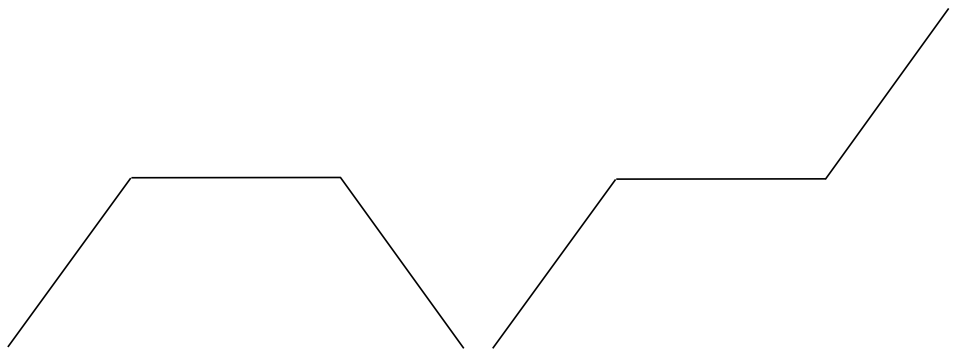
Recall that the *maximum span* of an open polygonal chain $(v_0, v_1, \ldots, v_n)$ is definied as the maximum distance between its endpoints v_0 and v_n achieved over all configurations of the chain. The *maximum flat span* of a chain is the largest such distance achieved in any flat configuration of the chain. A *flat configuration* of a chain is a configuration in which all links lie in one plane without self-intersection. The *minimum span* and *minimum flat span* are defined analogously.

Computing the minimum and maximum spans of a chain are of interest to polymer physicists, who often need to compute the distribution of the distances between the endpoints of a polymer [Sos01]. This is because the mean-squared distance between the endpoints of polymers relates to their physical properties such as light diffusion and scattering [Sos01]. We will also see, in Section 6 below, that the maximum span leads to bounds on the length ratio needed to lock a chain. This connection motivated our study of the maximum span.

As mentioned in the Introduction, Soss proved that computing the minimum or maximum flat span of a chain is NP-hard [Sos01]. Both proofs are by reduction from SET PARTITION.

Hardness of computing extreme spans in 3D remains open for general fixed-angle polygonal chains, but we'll show that for a specific class of these chains the problem becomes easy, requiring only a constant amount of computational time. This subclass is the class of unit α-chains. We'll also show, in Section 8.3, that the max span of non-unit $90°$-chains can be computed in $O(n^3)$ time. In order to prove our complexity results for the class of unit α-chains, we need to introduce some terminology imported from biochemists.

The *cis*-configuration of a molecule refers to the configuration where opposite groups lie on the same side with respect to a line of reference, as in Fig. 8(a), while *trans*-configuration of a molecule refers to the configuration where opposite groups lie on opposite sides with respect to a line of reference, as in Fig. 8(b) [MW97]. Although typically these terms refer to the location of opposite groups across a double bond (alkene), we will extend the terms analogously to describe polygonal chains. We define the *trans*-configuration of a fixed-angle chain as



(a) *Cis*-configuration. (b) *Trans*-configuration.

Figure 8:

the planar configuration in which the turns at each joint alternate between $+\tau_i$ and $-\tau_i$, where $\tau_i = \pi - \alpha_i$. We say that a configuration is *maximal* if the maximum span is achieved in this configuration.

Lemma 5.1 (3-Chain Lemma) *The maximum span of any fixed-angle 3-chain is achieved in a planar configuration.*

Proof: Let the chain be (v_0, v_1, v_2, v_3), and let β denote the angle between v_0v_2 and v_2v_3. Then the maximum distance between v_0 and v_3, $\max|v_0v_3|$, is achieved when β is largest, because the lengths $|v_0v_2|$ and $|v_2v_3|$ are already determined by the fixed edge lengths and fixed turn angles of the chain, leaving only β to vary. Now we just need to show that β is largest when v_3 is in the plane Π determined by $\{v_0, v_1, v_2\}$. See Fig. 9. If we look down on Π from above, we obtain the view shown in Fig. 10. It is clear that the red line, the projection of the cone rim on which v_3 rides (cf. Fig. 9), intersects each level curve at most once, beginning at some intermediate β and ending at the maximum β in the plane Π. Hence $\max|v_0v_3|$ is achieved when v_3 lies in Π, and so the maximal configuration is planar. □

Note that this lemma holds for arbitrary joint angles, not necessarily all equal, as does the next lemma.

Lemma 5.2 (4-Vertex Lemma) *Let $(v_0, v_1, v_2, \ldots, v_{k-2}, v_{k-1}, v_k)$ be a fixed-angle k-chain. Then in any maximal configuration of the chain, vertices $\{v_0, v_1, v_2, v_k\}$, and vertices $\{v_0, v_{k-2}, v_{k-1}, v_k\}$ are coplanar.*

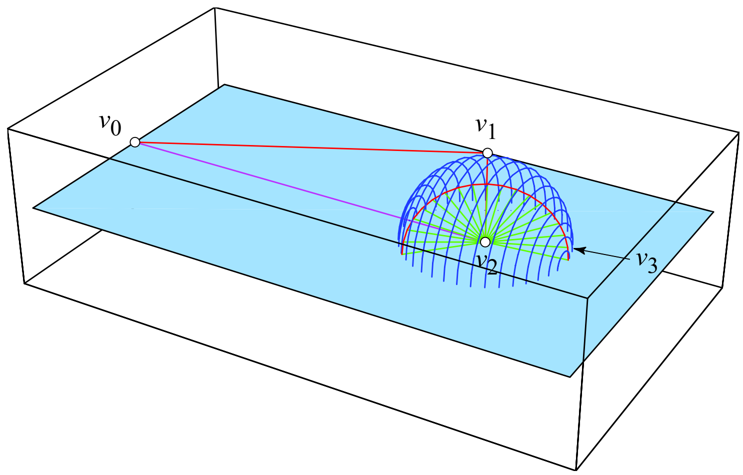


Figure 9: The maximum span of a 3-chain is achieved in a flat configuration. The blue rings are the level sets for β, where β is the angle between v_0v_2 and v_2v_3. The angles increase from left to right along the pink line. The green ribs specify all possible locations of edge v_2v_3, which rides along a cone whose axis is v_1v_2. The rim of the cone (red) is the locus of possible locations of v_3.

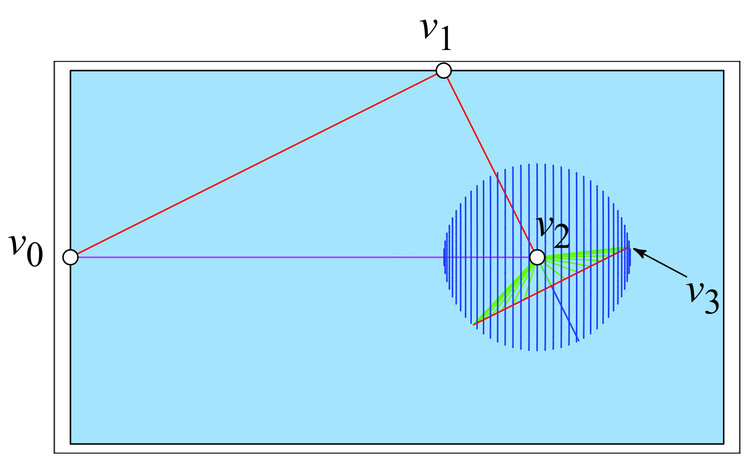


Figure 10: The red line intersects each level curve at most once, starting at some intermediate β (toward the left), and ending at the maximum β (toward the right) in the plane of $\{v_0, v_1, v_2\}$.

Proof: We prove the latter claim; the former follows by relabeling the vertices in reverse. Let Π be the plane determined by $\{v_0, v_{k-2}, v_{k-1}\}$. As in the proof of the 3-chain Lemma 5.1, let β denote the angle between v_0v_{k-1} and $v_{k-1}v_k$. Any position of the three vertices $\{v_0, v_{k-2}, v_{k-1}\}$ in Π determine a "virtual" 3-chain $(v_0, v_{k-2}, v_{k-1}, v_k)$ whose span is maximized when v_k lies in Π (i.e., when β is largest) by Lemma 5.1. That is to say, for any such position, rotating v_k into the planar *trans*-configuration of the corresponding 3-chain yields the largest distance between v_0 and v_k for those particular positions of the vertices v_0, v_{k-2}, and v_{k-1}. Hence, in any maximal configuration, we must have $\{v_0, v_{k-2}, v_{k-1}, v_k\}$ coplanar; otherwise we could increase the distance between v_0 and v_k by rotating v_k into Π. $\square$

5.1 Unit α-Chains

In the above lemma and corollary we made no assumptions on the link lengths, nor on the joint angles, except that both are fixed. Now we specialize to unit-length chains, all of whose angles are equal to α, i.e., unit α-chains. Our first lemma will serve as the base case in an induction proof to follow.

Lemma 5.3 *The maximum span of a unit α-chain of 4 links, is achieved in a planar configuration.*

Proof: Let $(v_0, v_1, v_2, v_3, v_4)$ be such a chain. Let Π be the plane determined by $\{v_0, v_1, v_2\}$. Draw a sphere of radius $|v_0v_2|$ centered at v_2. Because $|v_2v_4| = |v_0v_2| = 2\sin\frac{\alpha}{2}$, v_4 must also lie on this sphere. See Fig. 11. By Lemma 5.2, we know that v_4 must also lie in Π. Hence v_4 must lie on the "equatorial" great circle that is the intersection of Π with the sphere. The maximum distance between v_0 and v_4 is just the diameter of this circle, i.e., $|v_0v_2| + |v_2v_4| = 2|v_0v_2|$. And since the planar *trans*-configuration achieves this distance, we have that the maximal configuration is planar. See Fig. 12.

$\square$

We will see later (Facts 7.3 and 7.1) that this lemma is false without either the unit-length or the same-angle assumptions. However, there is no restriction on the fixed angle α.

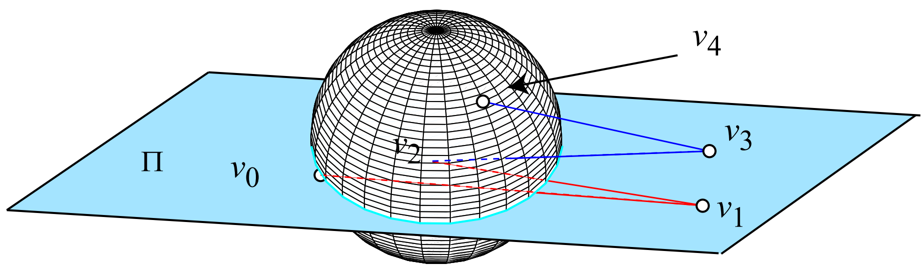


Figure 11: A sphere of radius $|v_0v_2|$ centered at v_2. Since $|v_2v_4| = |v_0v_2| = 2\sin\frac{\alpha}{2}$, v_4 must also lie on this sphere.

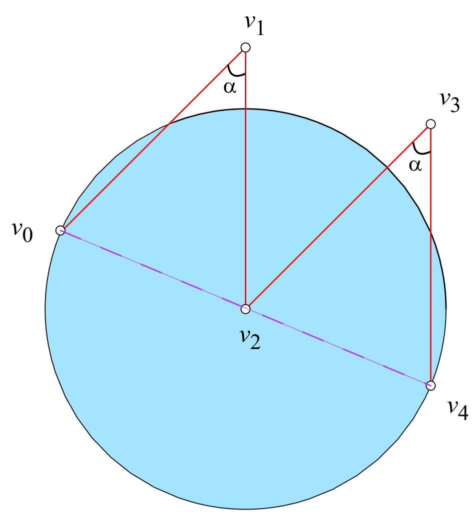


Figure 12: The maximal configuration of a unit, fixed-angle 4-chain with joint angles α is the *trans*-configuration. Notice that the span is just the diameter of the circle centered at v_2, which is equal to $2\,|v_0v_2|$.

We now focus on unit α-chains of an arbitrary number of links. The argument is different for even and odd number of links.

Lemma 5.4 *The maximum span of a unit α-chain, having an even number k of links, is achieved by the planar* trans-*configuration.*

Proof: We will prove this by induction. The base case $n = 4$ is achieved in the planar *trans*-configuration by Lemma 5.3 above. Assume true for all even $n \leq k-2$ that the maximal configuration of a unit α-chain with n links is the planar *trans*-configuration, i.e., $\max|v_0v_n|$ is achieved in the planar *trans*-configuration. Now we'll show that this is true for $n = k$ by using a subadditive argument.

Clearly,

$$\max|v_0v_k| \leq \max|v_0v_{k-2}| + |v_{k-2}v_k|$$

because the distance $|v_{k-2}v_k|$ is uniquely determined from the joint angle α and the unit lengths $|v_{k-2}v_{k-1}| = 1$ and $|v_{k-1}v_k| = 1$. (In other words, were $\max|v_0v_k|$ larger than this quantity, the fixed distance $|v_{k-2}v_k|$ would imply that $\max|v_0v_{k-2}|$ is not in fact maximal.) By induction, $\max|v_0v_{k-2}|$ is achieved in the planar *trans*-configuartion. The planar *trans*-configuration of the full k-chain gives us equality in the above expression, so this must be the maximal configuration since $|v_0v_k|$ can be no larger. See Fig. 13.

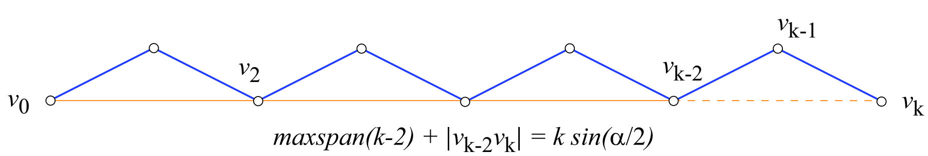


Figure 13: The maximal configuration of a unit, k-chain for even k (and joint angles all equal to α) is the planar *trans*-configuration.

$\square$

Lemma 5.5 *The maximum span of a unit α-chain, having an odd number k of links, is achieved in the planar* trans-*configuration.*

Proof: Proving this result for odd k is significantly more difficult, despite our intuition that the maximal configuration for odd k should also be the planar *trans*-configuration. We will again use induction. Our base case is a unit 3-chain, which we know we know has the planar *trans*-configuration for its maximal configuration by Lemma 5.1. Assume it is true for all odd $n \leq k-2$ that the maximal configuration of a unit n-chain with joint angles α is the planar *trans*-configuration. We'll now show true for $n = k$.

Let Π be the plane determined by vertices $\{v_{k-2}, v_{k-1}, v_k\}$. Now we will show that the position of v_0 that maximizes $|v_0 v_k|$ is that of the planar *trans*-configuration. By the 4-vertex Lemma 5.2, we know that v_0 must also lie in Π if we are to achieve a maximal configuration. Let maxspan $|m|$ denote the max span of a unit α-chain with m links. Let transspan $|m|$ denote the span of the *trans*-configuration of such a chain.

Draw a circle C_{k-2} of radius maxspan $|k-2|$ centered at v_{k-2}. We know by the induction hypothesis that this radius is just the span of the *trans*-configuration, that is, maxspan $|k-2|$ = transspan $|k-2|$. Similarly draw a circle C_{k-1} of radius maxspan $|k-1|$ centered at v_{k-1}. Now since $k-1$ is even, maxspan $|k-1|$ = transspan $|k-1|$ by Lemma 5.4. Finally, draw a circle C_k of radius transspan $|k|$ centered at v_k. It is clear that these three circles C_{k-2}, C_{k-1}, and C_k must intersect at a common point v^*, since any subchain of a *trans*-chain is itself *trans*, and all three circles are based on transspans. This construction is displayed in Fig. 14.

We aim to prove that the maxspan $|k|$ is achieved when $v_0 = v^*$. This v^* is the position of v_0 when $(v_0, \ldots, v_k)$ is in the *trans*-configuration. Suppose for contradiction that there is a position of v_0 for which $|v_0 v_k| > |v^* v_k|$. Then v_0 is exterior to C_k (blue circle in Fig. 14). Let L denote the line through v^* and v_k. If L also passes through v_{k-2}, then the last two links exactly extend the *trans*-configuration of the first $k-2$ links, and we are finished. So assume L misses v_{k-2}, and in particular, intersects $v_{k-2}v_{k-1}$.

That this intersection is without a loss of generality can be seen by the following reasoning. Orient the chain horizontally (that is to say, the x-axis bisects each link of the chain and so the y-coordinates of each vertex alternate between $+y$ and $-y$) as in Fig. 15 with v^* having y-coord $+y$. Both v_{k-2} and v_k have y-coord $-y$, and v_k lies to the right of v_{k-2}; hence the line L through $v^* v_k$ is above the line $v^* v_{k-2}$. And the y-coordinate of v_{k-1} is $+y$, so the line

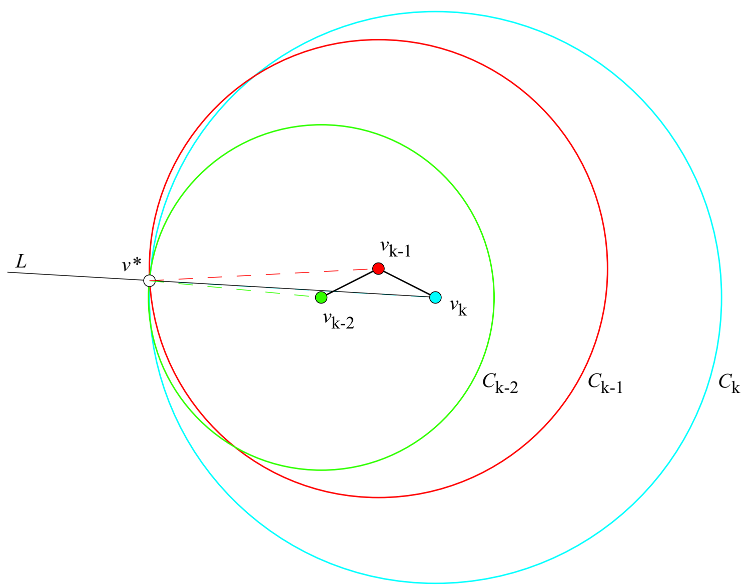


Figure 14: C_{k-2} is a circle of radius maxspan $|k-2|$ = transspan $|k-2|$ centered at v_{k-2}, C_{k-1} is a circle of radius maxspan $|k-1|$ = transspan $|k-1|$ centered at v_{k-1}, and C_k is a circle of radius transspan $|k|$ centered at v_k. The circles C_{k-2}, C_{k-1}, and C_k intersect at the common point v^*.

determined by v^*v_{k-1} is horizontal. Hence L is sandwiched between the lines along v^*v_{k-2} and v^*v_{k-1} and must intersect $v_{k-2}v_{k-1}$ by continuity.

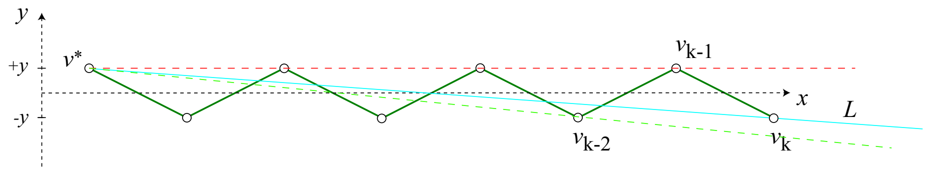


Figure 15: L must intersect $v_{k-2}v_{k-1}$.

We have two cases to consider.

Case 1: v_0 is above L and exterior to C_k. Because v_{k-2} lies below L and the radius of C_{k-2} is smaller than that of C_k, C_{k-2} (green in Fig. 14) lies interior to C_k above L. Hence, v_0 is exterior to C_{k-2}, which contradicts our assumption that maxspan $|k-2| =$ transspan $|k-2|$.

Case 2: v_0 is below L and exterior to C_k. Because v_{k-1} is positioned above L and the radius of C_{k-1} is smaller than that of C_k, C_{k-1} (red in Fig. 14) lies interior to C_k below L. Hence, v_0 is exterior to C_{k-1}, which contradicts our assumption that maxspan $|k-1| =$ transspan $|k-1|$.

Hence v_0 must lie interior or on the boundary of C_k. Thus we have

$$|v_0v_k| \leq |v^*v_k| = \text{transspan}\,|k|$$

so the maximum of $|v_0v_k|$ is achieved by taking $v_0 = v^*$. And since v^* corresponds to the planar *trans*-configuration of the k-chain, we have that the maximal configuratoin of the k-chain occuring in the *trans*-configuration as desired. $\square$

Putting Lemmas 5.4 and 5.5 together, we obtain:

Theorem 5.6 *The maximum span of any unit α-chain is achieved in the planar* trans-*configuration.*

Corollary 5.7 *Computing the maximum span for unit α-chains takes constant time.*

Proof: Let C be a unit α-chain with k links.

Case 1: The number of links k is even. Then the max span of C is simply

$$\frac{k}{2}|v_0v_2| = \frac{k}{2}\,2\sin\frac{\alpha}{2} = k\,\sin\frac{\alpha}{2},$$

where α is the joint angle of the chain. See Fig. 16. Notice the subadditivity of the max span in the case where k is even.

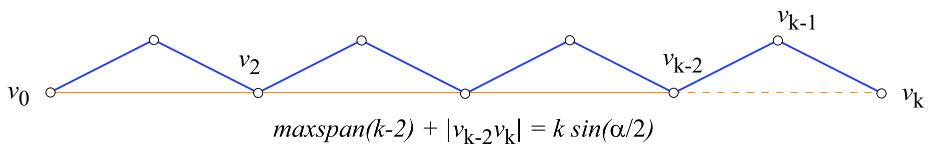


Figure 16: The maximal configuration of a unit, α-chain for even k is its *trans*-configuration. Its span is equal to $k\sin\frac{\alpha}{2}$.

Case 2: The number of links k is odd. Then the max span of C is the length of the hypotenuse of the shaded triangle in Fig. 17, which is

$$\sqrt{(k\sin\frac{\alpha}{2})^2 + \cos\frac{\alpha}{2}^2}.$$

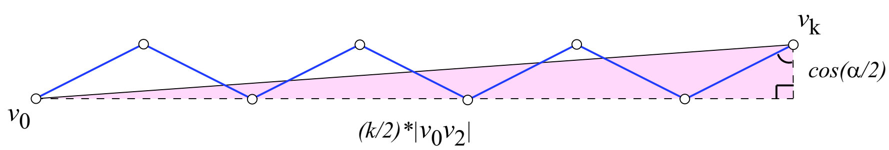


Figure 17: The maximal configuration of a unit, α-chain for odd k is its *trans*-configuration. Its span is just the length of the hypotenuse of the pink triangle.

□

The values of the max span $M(k, \alpha)$ for unit α-chains with k links are listed in Table 5.1. See Fig. 18 for a plot of the max span of unit α-chains as function

k	α	$M(k, \alpha)$
3	60°	1.73
4	90°	2.91
5	108°	4.09
6	120°	5.22
7	128.6°	6.32
8	135°	7.40

Table 1: The max spans of unit k-chains for various bond angles α and up to 8 links.

of k (up to $k = 10$) for $\alpha = 60°$, $90°$, and $135°$.

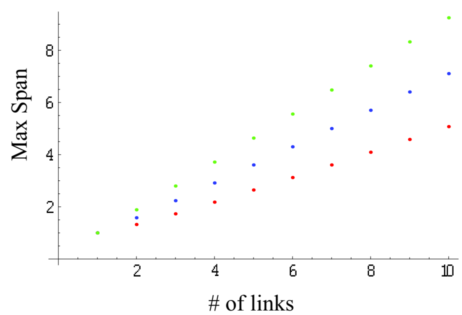


Figure 18: This plot shows the max span of unit α chains as a function of k (up to $k = 10$) for $\alpha = 60°$ (red), $90°$ (blue), $135°$ (green).

6 Connection between Locked Chains and Maximum Span [5]

The "knitting needles" example is a 5-chain with universal joints that is locked. See Fig. 19. It has three central unit links, and two end longer links. It is proved in [DO06, Thm. 6.3.1] that the chain is locked if the long links have length

[5]This section was first drafted by Joseph O'Rourke to provide motivation for our study of maxspans.

strictly greater than 3. The proof argues that if the long links are connected by a rope, then the resulting trefoil knot would be untied if the chain could be straightened. This contradiction establishes that the chain is locked.

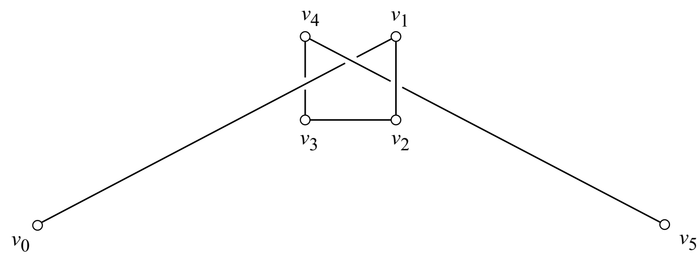


Figure 19: The knitting needles is an example of a locked 5-chain with universal joints

We establish here a (weak) connection between locked fixed-angle chains and the maximum span, which was our original motivation for exploring the span. Essentially it indicates the length ratio must be able to "overcome" to maximum span. First we observe this lemma:

Lemma 6.1 *Let C be a fixed-angle chain in some configuration, and J a subset of its joints. If C is locked when the joints in J are made universal joints, then C is locked when the joints in J are fixed-angle.*

Proof: Universal joints simply allow more freedom, so if they chain is stuck with universal joints, it is certainly stuck with fixed-angle joints. □

Now our strategy is to form a unit, regular, fixed-angle k-chain, add two links of length L weaving into a knitting-needles pattern, and follow the proof cited above to yield a lower bound on L which will ensure locking.

Theorem 6.2 *Let $n = k + 2$, and let $\alpha = \pi(k-2)/k = \pi(n-4)/(n-3)$ be the internal angle of a regular k-gon. Then there is a locked, near-unit, n-link α-chain, whose length ratio is $L = M + \epsilon$ (for any $\epsilon > 0$), where M is the maximum span of a $k = n - 2$ unit-chain with fixed angle α.*

We first illustrate the theorem for $n = 8$, $k = 6$. Then $\alpha = \pi(4/6) = 120°$, the angle of a regular hexagon. Referring to Table 5.1, $M(6, 120°) = \sqrt{109}/2 \approx 5.22$.

We can create an 8-chain based on a unit regular hexagon, that is locked for $L > 5.22$. See Fig. 20a.

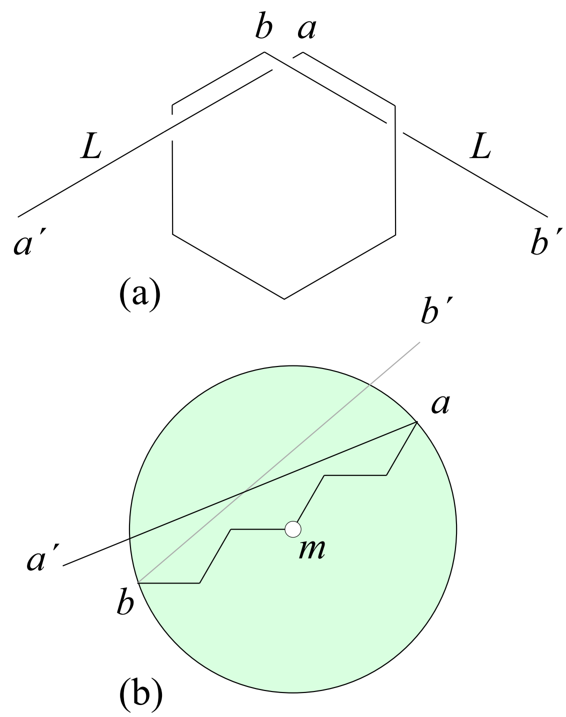


Figure 20: Locked 8-chain based on a unit regular hexagon.

Proof: Form the knitting-needles configuration as illustrated in Figure 20a for $k = 6$. We saw in Figs. 16 and 17 that the maximum span configuration of a unit k-chain is symmetric about the median point m of the chain, which is a vertex when k is even, and the midpoint of an edge when k is odd.

Draw a sphere S of diameter M centered on m. Connect the two endpoints a' and b' by a rope outside of S. Then, as in the proof in [DO06], unlocking the chain requires either a' or b' to enter S, for otherwise the rope maintains it in a trefoil knot. If we imagine joints a and b universal joints, then it is clear that $L > M$ will prevent that penetration; see Figure 20b. As all the short segments are confined inside S, and a' and b' excluded outside S, the chain remains locked. $\square$

We believe this result is weak. For example, for $n = 6$ and $k = 4$, $\alpha = 90°$, the theorem predicts $L > \sqrt{17/2} \approx 2.91$, but we know from Figure 6 [LO04] that $L = \sqrt{2} + \epsilon$ suffices to lock a 90° near-unit chain.

The reason for the weakness, we believe, is that treating a and b as universal joints loses a significant constraint. In fact the angle at those joints must be α as well (unlike the sharply acute angle drawn in Figure 20b). If we insist that all angles be α, then the relevant L is smaller, as indicated in Fig. 21. In effect, the

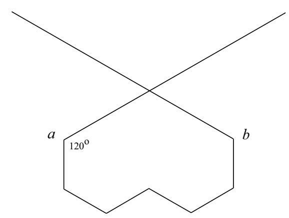


Figure 21: All joint angles α.

two extreme unit links are frozen, and the span determined by the remaining $k - 2$ links. A calculation shows that this yields exactly $L = \sqrt{2}$ for $n = 6$ and $\alpha = 90°$, but we do not know how to formalize these observations.

7 Nonplanar Maximal Span Configurations

Naturally one might ask whether the maximal configuration remains planar for non-unit chains with all equal joint angles, even special angles such as 90°, or for unit-chains with non-equal joint angles. The answer is NO in all three cases. Soss [Sos01] was the first to show that the maxspan of a 4-chain might be achieved in a nonplanar configuration. He provides an example of a 4-chain with acute angles whose maximal configuration is nonplanar. We provide other examples of chains with nonplanar maximal configurations in Figures 22, 23, and 24.

Fact 7.1 *The maximal configuration of an α-chain whose edge lengths are not all equal, is not necessarily planar.*

Proof: Fig. 22 gives an example of a non-unit chain, with equal joint angles whose maximal configuration is nonplanar. The lengths of the edges v_0v_1, v_1v_2,

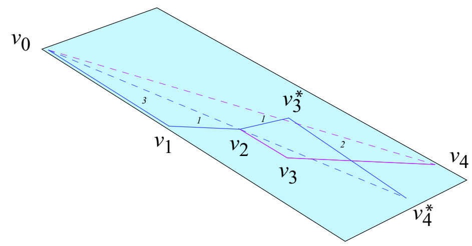


Figure 22: An example of a nonunit, α-chain whose maximal configuration is nonplanar. The span of the nonplanar configuration is 6.57, while the span of the planar configuration is 6.48.

v_2v_3, and v_3v_4 are 3,1, 1, and 2, respectively. The span of the nonplanar configuration is 6.57, while the span of the planar configuration is 6.48. $\square$

Even specializing to all angles equal to 90° does not guarantee planarity. See Fig. 23.

Fact 7.2 *The maximal configuration of a non-unit* $90°$*-chain is not necessarily planar.*

Proof: Fig. 23 gives an example of a non-unit 90° 4-chain, whose maximal configuration is nonplanar. The lengths of the edges v_0v_1,v_1v_2, v_2v_3, and v_3v_4 are 2, 1, 1, and 2, respectively. The span of the nonplanar configuration is ≈ 4.47, while the span of the planar configuration is ≈ 4.24.

$\square$

Fact 7.3 *The maximal configuration of a unit, fixed-angle chain whose joint angles are not all equal, is not necessarily planar.*

Proof: Fig. 24 gives an example of a unit chain, with nonequal joint angles whose maximal configuration is nonplanar. The length of each link is 1, and the angles at v_1, v_2, and v_3 are $\pi/2$,$\pi/2$, and $\pi/4$, respectively. The span of the nonplanar configuration is ≈ 2.18, while the span of the planar configuration is ≈ 2.17. $\square$

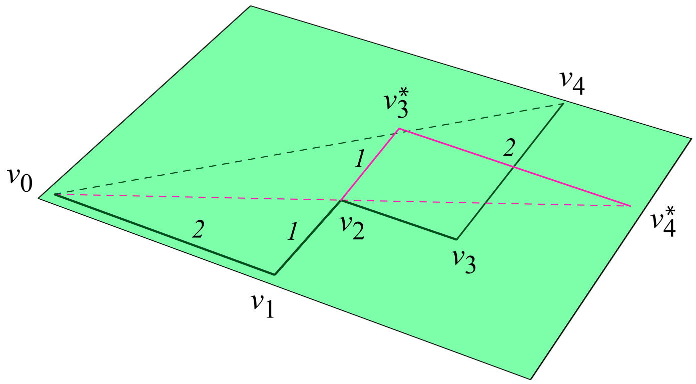


Figure 23: An example of a nonunit, 90° 4-chain whose maximal configuration is nonplanar. The nonplanar configuration has it's fourth and fifth vertices denoted as v_3^* and v_4^*, respectively. The span of the nonplanar configuration is ≈ 4.47, while the span of the planar configuration is ≈ 4.24.

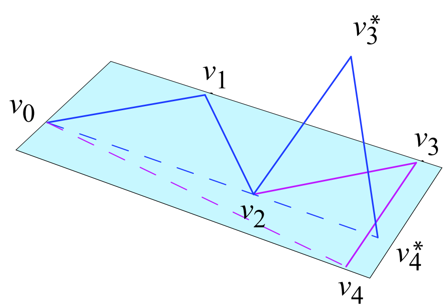


Figure 24: An example of a unit, fixed-angle chain with nonequal joint angles, whose maximal configuration is nonplanar. The span of the nonplanar configuration is ≈ 2.18, while the span of the planar configuration is ≈ 2.17.

7.1 Alignment Lemmas

Figs. 24 23 illustrate a nice property of 4-chains. Notice how the spans in both of these chains align, that is, the max span of the 4-chain is the sum of two 2-spans. Soss [Sos01] noticed this property in his example of a 4-chain with nonplanar maxspan, where he used collinearity of v_0, v_2, v_4 to argue that the span was indeed maximal.

For 4-chains, the maximal configuration can be achieved in one of two ways:

1. The spans of subchains $(v_0, v_1, v2)$ and (v_2, v_3, v_4) align. Hence the 4-span is the sum of two 2-spans.

2. The maximum span configuration is planar.

The following lemma shows that, if there is alignment of subchain maximum spans, then that realizes the maximum span of the full chain.

Lemma 7.1 *Let $C = (v_0, \ldots, v_n)$ be a fixed-angle n-chain. If there is a k such that the maximum span of $A = (v_0, \ldots, v_k)$ can (by the allowable joint angle at v_k) align with the maximum span of $B = (v_{k+1}, \ldots, v_n)$, then it must be that* $\text{maxspan}(C) = \text{maxspan}(A) + \text{maxspan}(B)$*, achieved by that alignment.*

Proof: In any configuration of C, we can identify a triangle $\triangle(v_0, v_k, v_n)$. By the triangle inequality, $|v_0v_n| \leq |v_0v_k| + |v_kv_n|$. and we know that $|v_0v_k| \leq \text{maxspan}(A)$ and $|v_kv_n| \leq \text{maxspan}(B)$. Therefore, $|v_0v_n| \leq \text{maxspan}(A) + \text{maxspan}(B)$. Hence, when this upper bound is achieved by alignment, it must be the maximum for the whole chain. □

7.2 4-chain Flower

Let $C = (v_0, v_1, v_2, v_3, v_4)$ be a fixed-angle 4-chain, and without a loss of generality pin down the first two links. We briefly characterize the locus of points where v_4 can lie. Even though we understand the possible maximum span configurations allowed for 4-chains (there are only two), computing this locus will be useful for the max span analysis in Subsection 7.3. Consider the sphere S of radius $|v_2v_4|$ centered at v_2. Then the locus of points where v_4 is permitted to lie is a region of the sphere bounded by two parallel planes, which are orthogonal to the axis v_1v_2. The top cutting plane comes from starting in the *trans*-configuration of the 3-chain (v_1, v_2, v_3, v_4), and then rotating the 2-chain (v_2, v_3, v_4) about the axis v_1v_2. The bottom cutting plane comes from starting in the *cis*-configuration of the 3-chain (v_1, v_2, v_3, v_4), and again rotating the 2-chain (v_2, v_3, v_4) about the axis v_1v_2. See Fig. 25.

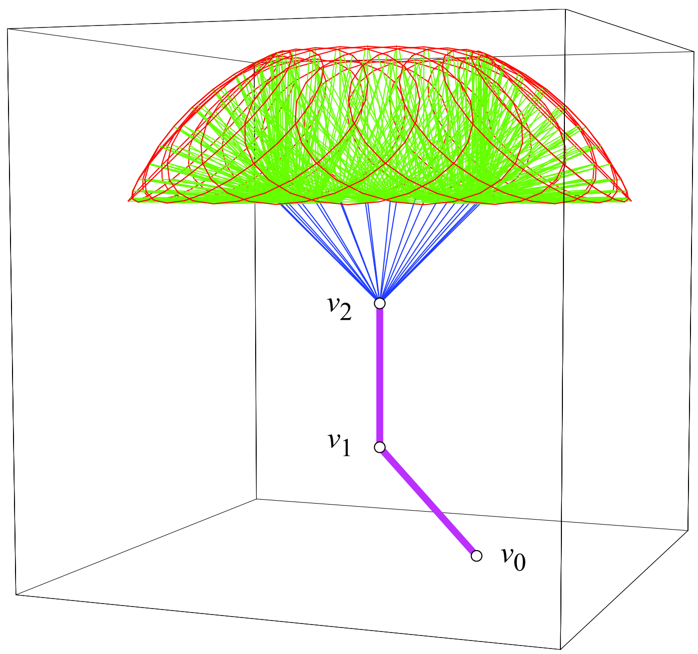


Figure 25: 4-chain flower for a unit 135°-chain.

7.3 90° 5-Chains

We now restrict our attention to 90° 5-chains for definiteness, although we believe the results extend to non-acute α (at the least). Indeed the remainder of the analysis in the thesis is restricted to $\alpha = 90°$. For the remainder of this section, we take v_0, v_1, v_2 to lie in the xy-plane. Recall that 4-vertex Lemma 5.2 guarantees the coplanarity of v_0, v_1, v_2, v_5 (as well as the coplanarity of v_0, v_3, v_4, v_5) in any maximal configuration. So in attempting to compute the max span of a 5-chain, we are only interested in configurations of the chain which place v_5 in the xy-plane.

As with the 4-chain, consider a sphere S of radius $|v_3v_5|$ centered at v_3. We know that v_5 is confined to a region of this sphere bounded by two parallel planes which are orthogonal to the axis v_2v_3. This is illustrated in Fig. 25 for $\alpha = 135°$ and Fig. 29 for $\alpha = 90°$. But before trying to understand the intersection of this region with the xy-plane, it is natural to ask what is the intersection of the whole sphere with the xy-plane. In other words, imagine a sphere centered at v_3 which itself lies on the rim of the cone whose axis is v_1v_2. (Note that, for $\alpha = 90°$, the "cone" degenerates to a disk.) We are asking for the intersection of this sphere with the xy-plane as v_2v_3 spins on its cone. It turns out that this sphere always intersects the plane in a coaxal family of circles, as shown in Fig. 26.

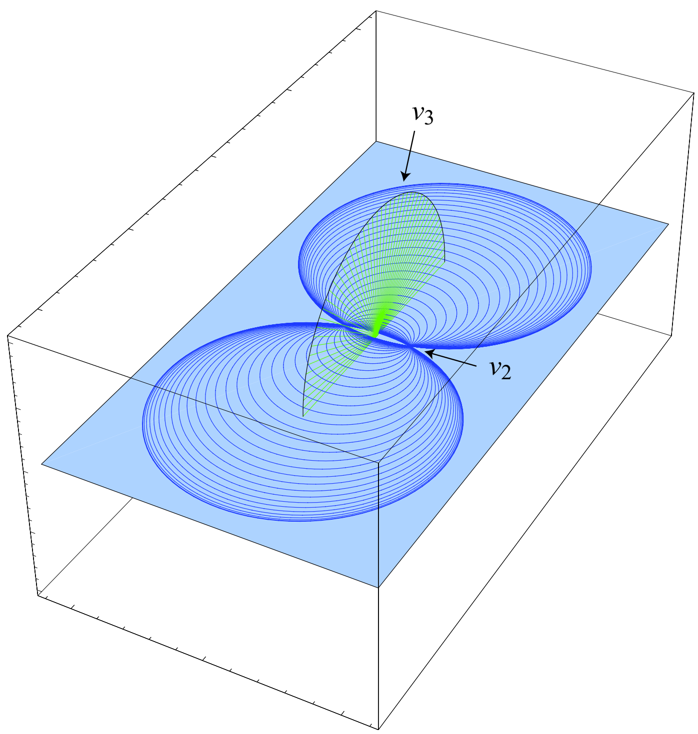


Figure 26: A sphere centered at v_3 intersects the xy-plane in a coaxal family of circles (blue) as v_2v_3 spins on its cone/disk (green).

Now since v_5 is confined to a region of the sphere truncated by two planes, the locus of points for v_5 in the xy-plane is a subset of the coaxal family of circles. Without a loss of generality, take v_0 to lie in the lower half of the xy-plane depicted in Fig. 27. Because we are trying to maximize $|v_0v_5|$, we are only interested in configurations which place v_5 in the upper half plane (since we've taken v_0 to lie in the lower half plane). Hence we may ignore the bottom half of the figure. The region corresponding to configurations that place v_5 in the xy-plane is a quadrilateral consisting of four arcs of circle. This quadrilateral is the intersection of the band of the sphere shown in Fig. 29 with the xy-plane as the sphere rotates around the v_3 rim shown in Fig. 26. The top arc ab is an arc of radius maxspan(v_2, v_3, v_4, v_5) centered at v_2, which happens to be the span the *trans*-configuration of this 3-chain. The bottom arc cd is an arc of the circle of radius minspan(v_2, v_3, v_4, v_5) centered at v_2, which is the *cis*-span of this 3-chain. The vertex v_5 is subject to the constraint that $|v_2v_5|$ is at least the min span of (v_2, v_3, v_4, v_5) and no greater than the max span of this 3-chain, which is what the top and bottom arcs represent. When v_5 lies along the left or right side arcs (bc and ad of Fig. 27), v_2v_3 lies in the xy-plane so the sphere centered at v_3 is cut in half and intersects the plane in a great circle. Hence arcs bc and ad are arcs of a great circle of this sphere, which recall has radius $|v_3v_5|$.

Let us now examine what it means for v_5 to lie on any one of these 4 arcs with respect to the max span. Because we have taken v_0 to lie in the lower half-plane, and are trying to maximize the span of the 5-chain, we know that v_5 must lie on the boundary of this quadrilateral. In particular, v_5 must lie along ab, bc, or ad in any maximal configuration of the 5-chain, for if it were strictly interior to the quadrilateral, a greater span could be achieved by moving to the boundary of the quadrilateral. If v_5 lies interior to the top arc ab, then we must have v_0v_5 orthogonal to ab for maximality–non-orthogonality would permit lengthening the span by moving toward orthogonality. Hence, v_0v_5 must pass through v_2, the center of this circle (this is the case illustrated in the figure). This alignment yields

$$|v_0v_5| = |v_0v_2| + |v_2v_5| = \text{maxspan}(v_0, v_1, v_2) + \text{maxspan}(v_2, v_3, v_4, v_5).$$

In other words, the max span is achieved by alignment of a 2-span plus a 3-span. This case is illustrated in Fig. 28.

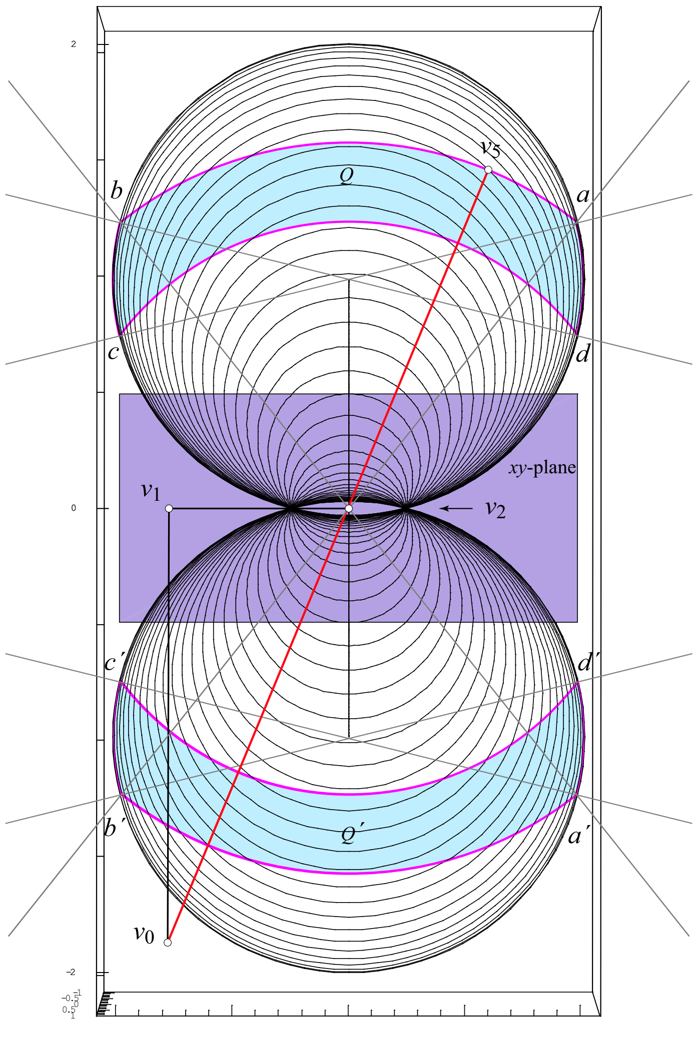


Figure 27: The region corresponding to configurations which place v_5 in the plane is a quadrilateral (blue region). The sides of the quadrilateral correspond to 4-arcs of circle. The top arc ab (pink) is an arc of the circle of radius maxspan(v_2, v_3, v_4, v_5) centered at v_2, which corresponds to the *trans*-configuration of this 3-chain. The bottom arc cd (also pink) is an arc of the circle of radius minspan(v_2, v_3, v_4, v_5) centered at v_2, which corresponds to the *cis*-configuration of this 3-chain. The side arcs ad and bc are arcs of a great circle of the sphere with radius $|v_3v_5|$. In this example, the link lengths of the 3-chain (v_2, v_3, v_4, v_5) are $(1, 1, \frac{1}{4})$.

Because bc and ad are symmetric, we'll only consider what happens if v_5 lies on one of these arcs, say ad. Suppose v_5 lies interior to ad. Then v_0v_5 is orthogonal to ad. Recall that ad corresponds to v_3 lying in the xy-plane, and so orthogonality implies that v_0v_5 pass through v_3. Also, recall that we have taken v_0, v_1, v_2 to lie in the xy-plane, so the additional coplanarity of v_3 implies that the 3-chain (v_0, v_1, v_2, v_3) is in its *trans*-configuration and hence achieves its max span. So we have,

$$|v_0v_5| = |v_0v_3| + |v_3v_5| = \text{maxspan}(v_0, v_1, v_2, v_3) + \text{maxspan}(v_3, v_4, v_5).$$

The only case left to consider is when v_5 lies at a corner (either b or a). Suppose v_5 lies at the corner $a = ba \cap ad$, and that v_0v_5 is orthogonal to neither ba nor ad (otherwise one of the above two cases would apply). Now since, v_5 lies along ad, we have v_3 lying in the xy-plane. Combining this fact with Lemma 5.2, we have coplanarity of v_0, v_1, v_2, v_3, v_5, as well as coplanarity of v_0, v_3, v_4, v_5. Now by our assumption that v_0v_5 is not orthogonal to ba or ad, we do not have collinearity of v_0, v_2, v_5 or v_0, v_3, v_5. Hence, we conclude that v_0, v_3, v_5 uniquely determine a plane, moreover since v_0, v_1, v_2 lie in the xy-plane, all vertices must lie in the xy-plane (i.e., the maximal configuration of the 5-chain is planar.)

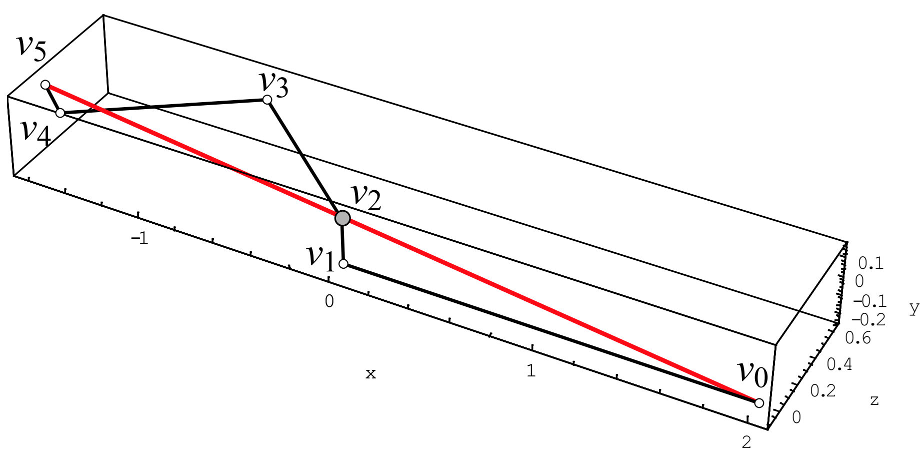


Figure 28: The maximum span (red) of a 90° 5-chain with link lengths $(2, \frac{1}{4}, 1, 1, \frac{1}{4})$. The last three links correspond to Fig. 27

We conclude this analysis with a summarizing theorem:

Theorem 7.2 *The maximum span of a* $90°$ 5*-chain is achieved in one of three configurations:*

1. *Alignment of the maximum spans of the* 2*-chain* (v_0, v_1, v_2) *and the* 3*-chain* (v_2, v_3, v_4, v_5)*, both in* trans*-configuration.*

2. *Alignment of the maximum spans of the* 3*-chain* (v_0, v_1, v_2, v_3) *and the* 2*-chain* (v_3, v_4, v_5)*, both in* trans*-configuration.*

3. *The* trans*-configuration of the full* 5*-chain.*

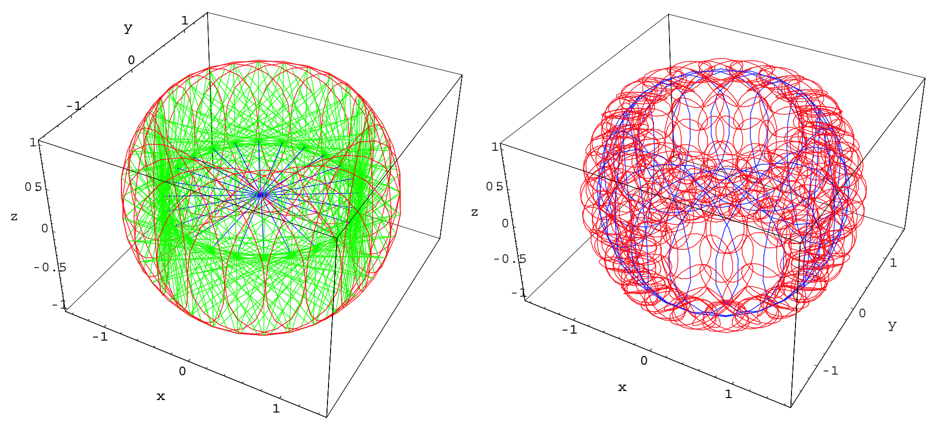


Figure 29: This figure depicts a 2-chain torus/flower (left) generated by link lengths $(1, 1)$, and a 3-chain torus/flower (right) generated by lengths $(1, 1, \frac{1}{4})$, both for $\alpha = 90°$. The right figure corresponds to the quadrilaterals in Fig. 27, although oriented differently: v_5 lies on the red circles, which intersect the xz-plane in two quadrilaterals.

8 The Maximum Span of n-link $90°$-Chains

8.1 Gradient Ascent Examples

We now generalize Theorem 7.2. The generalization was suggested by a program written by Joseph O'Rourke which found the maximum span configurations of

n-link chains empirically by gradient ascent. We will not discuss this program further, but some of its outputs are shown in Figs. 30-35. It was these empirical results that suggested the main structural theorem we prove in Theorem 8.4 below.

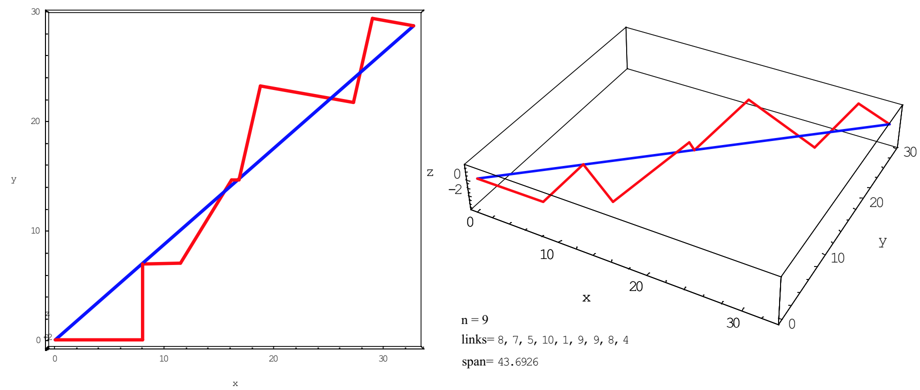


Figure 30: Two views of a 9-chain: $2 + 3 + 4$ subchains.

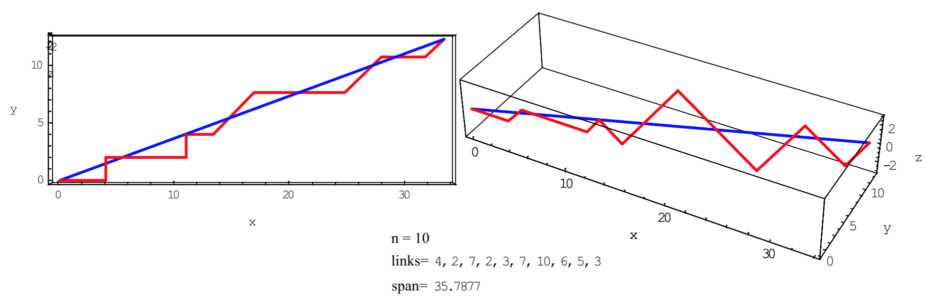


Figure 31:

Figure 32: Two views of a 10-chain: $4 + 6$ subchains.

8.2 Structure Theorem [6]

We continue to specialize all analysis to $\alpha = 90°$.

[6]From this section onward, the results reported were obtained in direct collaboration with Joseph O'Rourke.

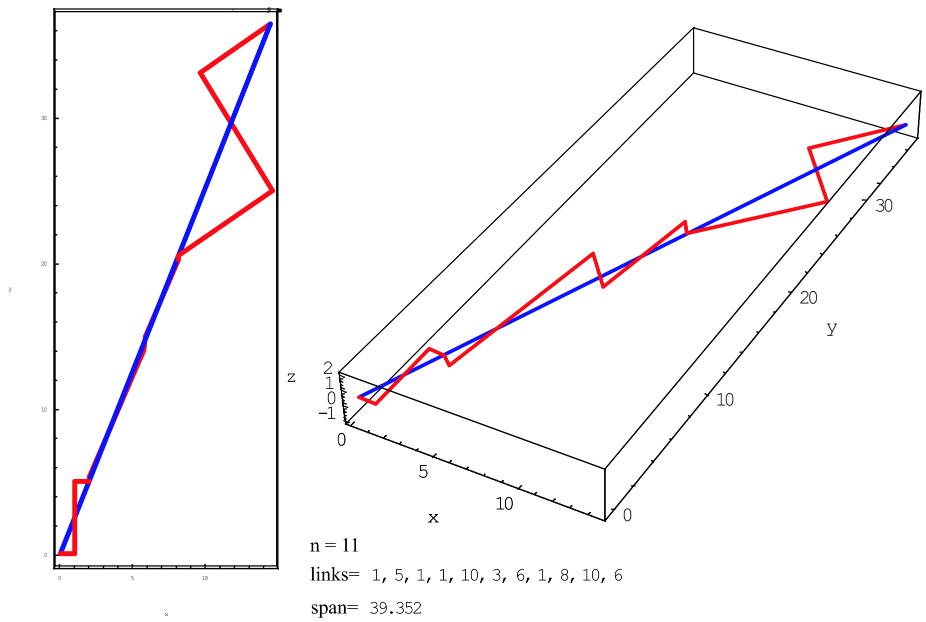


Figure 33: Two views of a 11-chain: $3 + 5 + 3$ subchains.

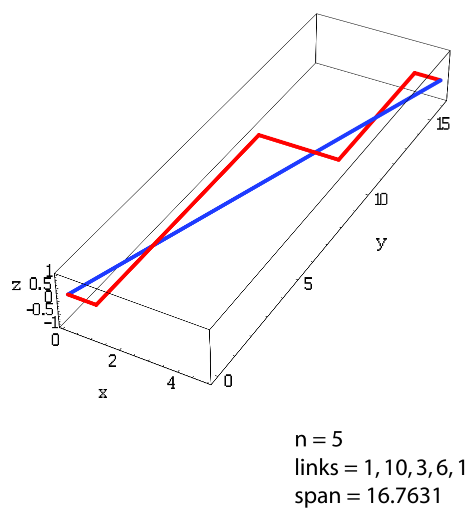


Figure 34: Testing that the span of the 5-chain contained in the $n = 11$ example (Fig. 33) is indeed its max span.

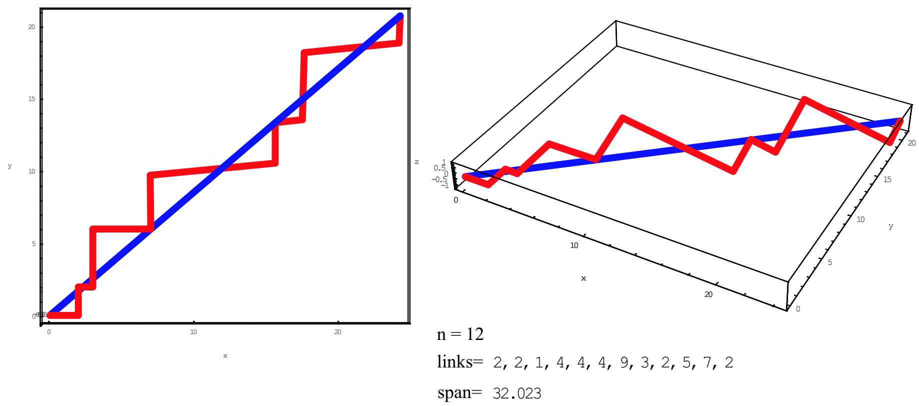


Figure 35: Two views of a 12-chain: $2 + 3 + 3 + 4$ subchains.

Lemma 8.1 *Let $C = (v_0, v_1, \ldots, v_n)$ be a chain that consists of several planar sections, and such that v_k is the first vertex at the joint between two planar sections where the span of $C_1 = (v_0, v_1, \ldots, v_k)$ is not aligned with the span of $C_2 = (v_k, v_{k+1}, \ldots, v_n)$. Then C cannot be in maximal span configuration.*

Proof: Suppose for contradiction that C is in its maximal span configuration. Let Π_0 be the plane determined by $\{v_0, v_1, v_2\}$, Π_1 be the plane determined by $\{v_0, v_{k-1}, v_k\}$, and Π_2 be the plane determined by $\{v_k, v_{k+1}, v_n\}$. First note that, because the sections up to v_k have their spans aligned, those spans all lie along the line L containing $v_0 v_k$, and each plane for each section includes L. Now, by assumption, v_{k+1} does not lie in Π_1; therefore $\Pi_1 \neq \Pi_2$. We will now show that either v_n lies along L, or $\Pi_1 = \Pi_2$, contradicting the assumptions of the lemma.

We replace C_1 with a 3-chain $C_1' = (v_0, u, v_{k-1}, v_k)$ lying in Π_1; and we replace C_2 with a 3-chain $C_2' = (v_k, v_{k+1}, w, v_n)$ lying in Π_2. The two replacements are performed by the same method, and we only explain the latter, illusrated in Fig. 36. Extend a ray from v_{k+1}, perpendicular to $v_k v_{k+1}$. Let w be the projection of v_n onto this ray. Then (v_k, v_{k+1}, w, v_n) is a 90° 3-chain. Let $C' = C_1' \cup C_2'$. Notice that we have not changed any spans; in particular, $\mathrm{span}(C') = \mathrm{span}(C)$.

Because C is in a maxspan configuration by hypothesis, we know (by the 4-Vertex Lemma 5.2) that v_n must lie in Π_0. And, again applying the 4-Vertex

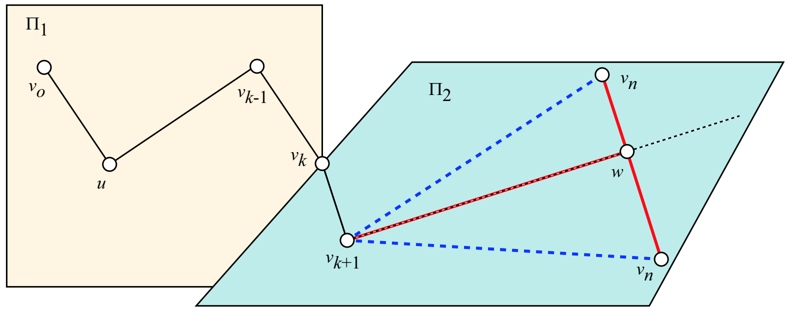


Figure 36: We replace C_1 with a 3-chain $C_1' = (v_0, u, v_{k-1}, v_k)$ lying in Π_1 by introducing u, and C_2 with a 3-chain $C_2' = (v_k, v_{k+1}, w, v_n)$ lying in Π_2 by introducing w. Two possible positions for v_n are shown.

Lemma, v_n must lie in Π_1, the plane determined by $\{v_0, u, v_{k-1}\}$. This leaves us with two cases to consider: either $\Pi_0 \neq \Pi_1$ or $\Pi_0 = \Pi_1$. We'll show that both cases lead us to a contradiction.

Case 1: Suppose $\Pi_0 \neq \Pi_1$. Then v_n lies along $L = \Pi_0 \cap \Pi_1$, contradicting the assumption that v_0, v_k, v_n are not aligned (else we'd have span(C_1) aligned with span(C_2)).

Case 2: Suppose $\Pi_0 = \Pi_1$. We now reason in a manner similar to that used for the suffix 3-chain of a 5-chain in Section 7.3 and Theorem 7.2. We have a suffix 3-chain C_2' at v_k, so v_n lies in or on the boundary of one of the two quadrilaterals Q or Q' identified in Fig. 27. By symmetry we may consider locations for v_0 in a quadrant of Π_1, with $v_n \in Q$. Refer to Fig. 37. Because C' is in its maximum span configuration, v_n must lie along arc ab or arc ad (taking v_0 to be in the shaded quadrant of Fig. 37). Now we claim that the only viable location for v_n is at the corner a. For suppose v_n were at some point p interior to arc ab. Arc ab is a smooth, differentiable curve (it is an arc of a circle), so v_0v_n must be orthogonal to ab because its distance is a maximum at p. Hence v_0v_n passes through the center of the circle containing arc ab, namely v_k. But this contradicts our assumption that v_0, v_k, v_n are not aligned. Similarly if v_n lies interior to arc ad, we get a contradiction. For completeness, we will go through this reasoning as well. The locus of points interior to arc ad correspond to configurations of C_2' having v_{k+1} lying in Π_1. And by our assumption the

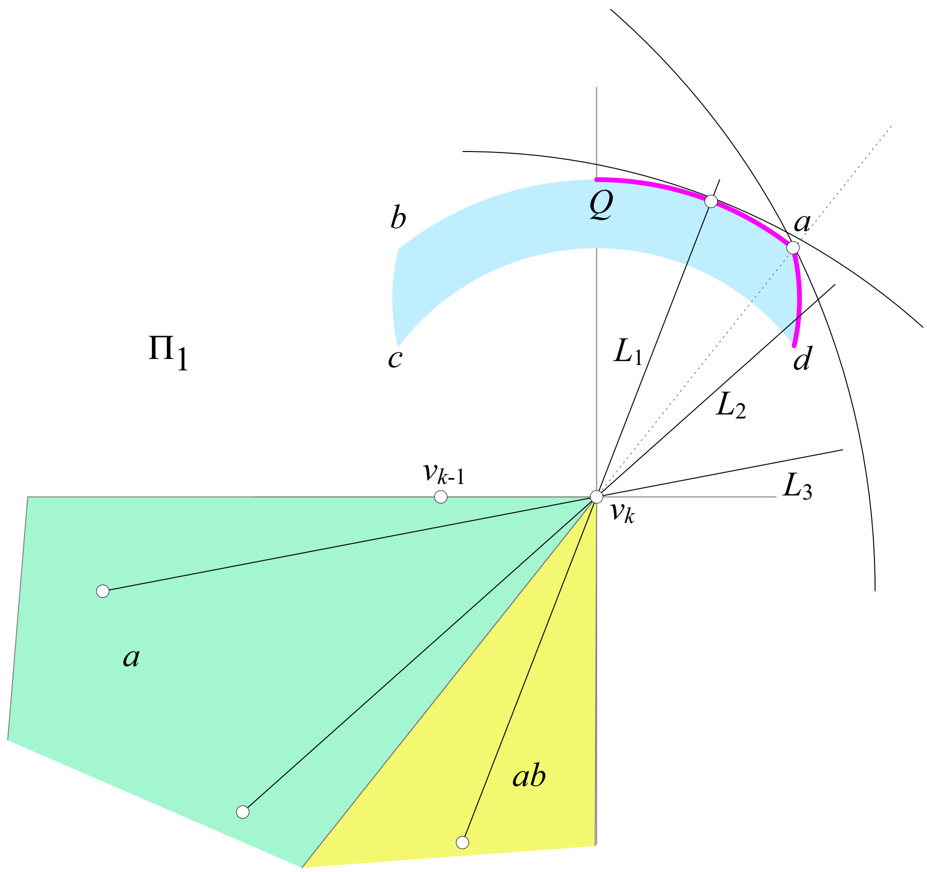


Figure 37: Q is the set of points where v_n might lie on Π_1. L_1, L_2, and L_3 are three possible lines of alignment. C' can be lengthened by placing v_n on ab (L_1) or at a (L_2 and L_3).

link $v_k v_{k+1}$ does not lie in Π_1.

Hence v_n must lie at the corner a of arcs ab and ad. But this point corresponds to the situation when the entire chain C'_2 is lies in Π_1 in its *trans*-configuration, which again contradicts our assumption that $\Pi_1 \neq \Pi_2$. Thus we conclude that the spans of any two distinct planar sections must align. In particular, if C is a chain that consists of several planar sections containing chains C_i, then the intersection of these planes is the line $v_0 v_n$ which passes through the start point and endpoint of every C_i.

□

Corollary 8.2 *In a maximal span configuration, the spans of each planar section must align, along the line segment* $v_0 v_n$*.*

Proof: Suppose there is some v_k at the joint between two planar sections of a chain C that does not lie on $v_0 v_n$; select the first such v_k. Then, if we partition C into C_1 and C_2 as above, then the spans of C_1 and C_2 do not align. Therefore the lemma shows that C could not be in maxspan configuration. □

Lemma 8.3 *If a chain is in maximal span configuration, each planar section must be in* trans-*configuration.*

Proof: Let $C = (v_0, v_1, \ldots, v_n)$ be a chain in its maximal span configuration. Suppose for contradiction that one of its planar sections contains a chain in its *cis*-configuration. Without a loss of generality, we may take such a chain to be a 3-chain C_i=$(v_k, v_{k+1}, v_{k+2}, v_{k+3})$, since we can always replace a chain consisting of several links with a 3-chain without changing the joint angles at its two endpoints or its span. See Fig. 38. Let L denote the line of alignment through $v_0 v_n$. We'll show that rotating $(v_k, v_{k+1}, v_{k+2}, v_{k+3})$ into its *trans*-configuration yields a new line of alignment L' and that the span of C is increased by this reconfiguration, contrary to our assumption that C was in its maximal span configuration.

Let $C_{i+1} = (v_{k+3}, \ldots, v_m)$ be the chain lying in the planar section after C_i. By Lemma 8.1, the endpoints of C_{i+1} lie along L. We temporarily replace $(v_{k+2}, v_{k+3}, \ldots, v_m)$ with a $90°$ 2-chain (v_{k+2}, u, v_m) by adding a vertex u along the line through $v_{k+2} v_{k+3}$ whose position is chosen such that $v_{k+2} u$ is orthogonal to v_m. Refer to Fig. 38. Notice that we have not changed the distance between

v_k and v_m. Let θ denote the angle between $v_k v_m$ and $v_k v_{k+1}$. We have two

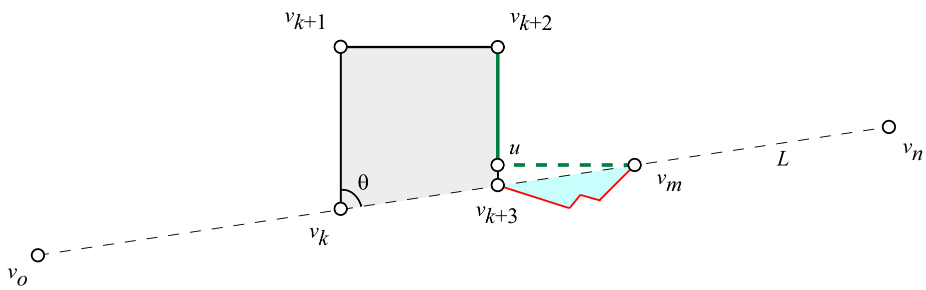


Figure 38: We temporarily replace $(v_{k+2}, v_{k+3}, \ldots, v_m)$ with a $90°$ 2-chain (v_{k+2}, u, v_m) by adding a vertex u along the line through $v_{k+2}v_{k+3}$ whose position is chosen such that $v_{k+2}u$ is orthogonal to v_m. This construction preserves the distance between v_k and v_m, as well as angles.

cases to consider.

Case 1: Suppose $\theta < \frac{\pi}{2}$. Rotate the *cis* 3-chain $(v_k, v_{k+1}, v_{k+2}, u)$ into the *trans*-configuration $(v_k, v_{k+1}, v_{k+2}, u')$, as shown in Fig. 40. Then the projection of v'_m onto L lies to the right of v_m, since $\theta < \frac{\pi}{2}$. So $v_0 v'_m$ is the hypotenuse of the right triangle with sides $v_0 v_m$, $v_m v'_m$. Hence $|v_0 v'_m| > |v_0 v_m|$. We rigidly join the rest of the chain $(v_{m+1}, \ldots, v_n)$ to v'_m such that v'_n lies along $v_0 v'_m$ and $|v'_m v'_n| = |v_m v_n|$. Let L' denote the new line of alignment through $v_0 v'_m v'_n$.

We have

$$\begin{aligned} |v_0 v'_n| = |v_0 v'_m| + |v'_m v'_n| &= |v_0 v'_m| + |v_m v_n| \\ &> |v_0 v_m| + |v_m v_n| = |v_0 v_n|, \end{aligned}$$

contradicting our assumption that C was in its maximum span configuration.

Case 2: If $\theta > \frac{\pi}{2}$, then flip $(v_{k+1}, v_{k+2}, \ldots, v_n)$ to the other side of L, as illustrated in Fig. 39, so that you are now in Case 1. And now the previous argument holds. $\square$

Theorem 8.4 (Structure Theorem) *The maximum span configuration for a* $90°$*-chain is either:*

1. *planar:* trans-*configuration*

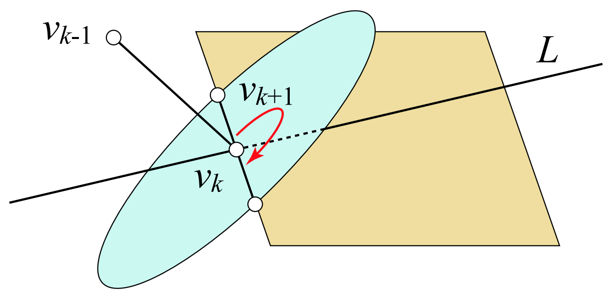


Figure 39: It is always possible to flip v_{k+1} to return to the same plane, while maintaining orthogonality with $v_{k-1}v_k$.

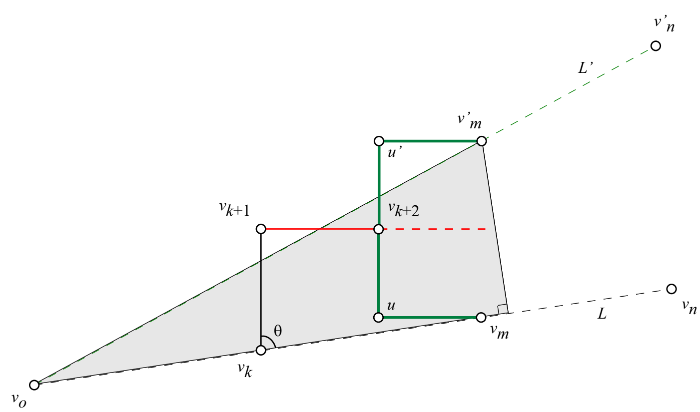


Figure 40: Rotating the *cis* 3-chain $(v_k, v_{k+1}, v_{k+2}, u)$ into the *trans*-configuration $(v_k, v_{k+1}, v_{k+2}, u')$ increases the span $|v_0 v_n|$ of the entire chain.

2. *nonplanar: there is a partition of the chain into planar sections, each of which:*

   (a) *is in maxspan* trans-*configuration; and*

   (b) *whose spans align*

This theorem captures the experimental results displayed in Figs. 30-35.

8.3 Dynamic Programming Algorithm

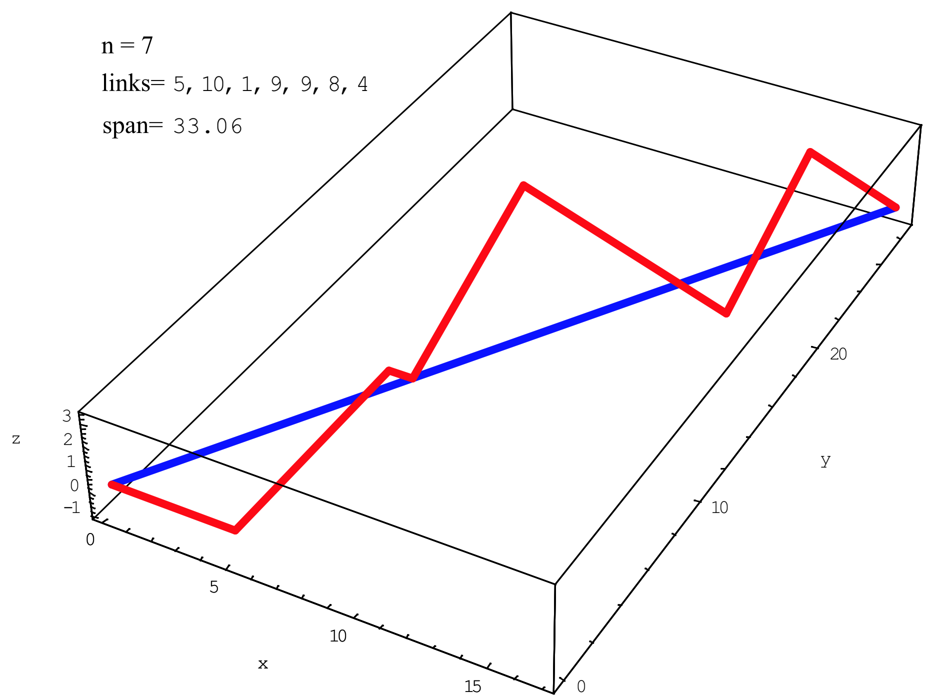


Figure 41: A 7-chain used to illustrate the dynamic programming algorithm.

In general, hardness of computing the maximum span in 3D is not known. However, we show that for 90°-chains it can be computed in $O(n^3)$ time via a dynamic programming algorithm.

Subchain	Details			
$2-chains$	$(5,10)$	$(1,9)$	$(9,9)$	$(8,4)$
span	11.2	9.1	12.7	8.9
$3-chains$	$(5,10,1)$	$(1,9,9)$		$(9,8,4)$
span	11.6	13.5		15.3
$4-chains$	$(5,10,1,9)$		$(9,9,8,4)$	
span	19.9		21.4	
$5-chains$	$(5,10,1)+(9,9)$		$(1,9,9,8,4)$	
span	$11.6+12.7=24.4$		22.0	
$7-chain$	$(5,10,1)+(9,9,8,4)$			
span	$11.6+21.4=33.1$			

Table 2: Dynamic programming table for chain with lengths $(5,10,1,9,9,8,4)$. Spans are reported to one decimal place.

Dynamic programming is a way of solving a problem by breaking it into subproblems, solving each subproblem which may have overlapping subsubproblems, and then combining these solutions [CLR90]. This strategy is typically applied to optimization problems [CLR90], such as finding the max span. Dynamic programming algorithms can greatly reduce the computational time required for a problem. By solving each subsubproblem exactly once, from smallest to largest, and storing the answer in a table, whenever a subsubproblem is subsequently encountered its solution does not need to be recomputed (just look up the answer in the table–this takes constant time) [CLR90].

The Structure Theorem 8.4 permits the 3D max span of 90°-chains to be found via a dynamic programming algorithm in polynomial time. We illustrate the steps of the algorithm for a 90° 7-chain example.

Steps of Algorithm on Example. First notice that a maximum span configuration will not have the first or last link constituting its own planar section. This is because if the first or last link constituted its own planar sectoin, then that link would have to lie along the line of alignment, and hence it would lie in the adjacent planar section (so considering it would be computationally redundant).

The following show the steps of the algorithm running on the example shown in Fig. 41. Refer to Table 8.3 throughout.

2. Compute the span of all 2-chains as the hypotenuse of the right triangle whose sides are the two links. The chains $(10, 1)$ and $(9, 8)$ are not included because they leave 1-chains at either end, so there are four relevant 2-chains.

3. Compute the span of all 3-chains; there are three. We know from Lemma 5.1 that the max span is achieved by the planar *trans*-configuration. The chains $(10, 1, 9)$ and $(9, 9, 8)$ are not included.

4. Compute the span of all 4-chains; there are two. The spans of $(5, 10)$ and $(1, 9)$ cannot align, so the max span of $(5, 10, 1, 9)$ is achieved by the planar *trans*-configuration. Similarly, the spans of $(9, 9)$ and $(8, 4)$ cannot align.

5. Compute the span of all 5-chains; there are two. For $(5, 10, 1, 9, 9)$, the subchains $(5, 10)$ and $(1, 9, 9)$ cannot align, but the subchains $(5, 10, 1)$ and $(9, 9)$ can align, and by Lemma 7.1, that realizes the max span as the sum of the spans of these two chains. For $(1, 9, 9, 8, 4)$, neither $(1, 9)$ and $(9, 8, 4)$ can align, nor can $(1, 9, 9)$ and $(8, 4)$, so the max span is achieved by the planar *trans*-configuration of the 5-chain.

6. Both 6-chains leave one link, and so need not be explored.

7. Finally, the complete 7-chain has partitions into $2 + 5$, $3 + 4$, $4 + 3$, and $5 + 2$ links. For example, the partition $(5, 10, 1, 9) + (9, 8, 4)$ would achieve a length of $19.9 + 15.3 = 35.2$, but in fact these cannot align. The only alignment is achieved by the partition $(5, 10, 1) + (9, 9, 8, 4)$, leading to a max span of $11.6 + 21.4 = 33.1$.

We analyze the steps above for an arbitrary $90°$ n-chain. By Lemma 8.3, each planar section is in its *trans*-configuration, so computing the max span of each subchain a constant time computation. Similarly, checking for the possibility of subchain $C_1 = (v_0, v_1, \ldots, v_{k-1}, v_k)$ aligning with subchain $C_2 =$

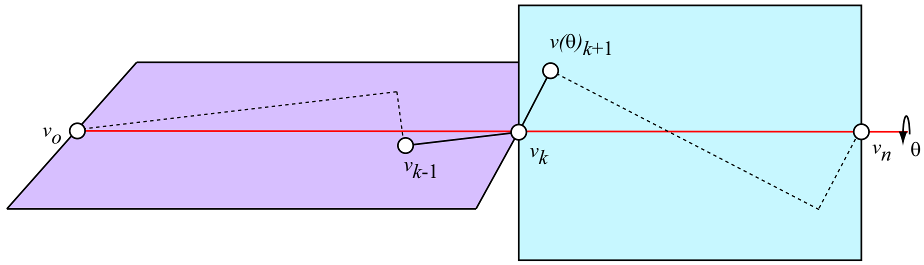


Figure 42: Spin the plane of C_2 about the line through $\{v_0, v_k, v_n\}$, and determine, if for any θ, $v_{k-1}v_k$ is orthogonal to v_kv_{k+1}.

$(v_k, v_{k+1}, \ldots, v_n)$ takes constant time, by the following argument. Simply attach C_2 to C_1 such that the line of alignment v_0v_k is collinear with the line of alignment v_kv_n. Then spin the plane of C_2 about the line through $\{v_0, v_k, v_n\}$, and see if at any point $v_{k-1}v_k$ is orthogonal to v_kv_{k+1}. See Fig. 42. If we parametrize the spin by θ, then this is equivalent to determining whether there exists a θ such that

$$(v_{k-1} - v_k) \cdot (v_{k+1}(\theta) - v_k) = 0,$$

a constant time computation.

There are $O(n)$ steps in each row and the table size is at most n^2, so the max span can be computed in $O(n^3)$ time.

9 Conclusion

Fixed-angle polygonal chains are of interest to the biochemical and physical community, because these chains can model the geometry of protein backbones [ST00] [DLO05], as well as polymers [Sos01]. This thesis investigated two properties of fixed-angle polygonal chains: (1) conditions for locking near-unit chains, and bounds on length ratios when the precise conditions seem inaccessible; (2) the *maximum span* of a chain, that is, the largest distance achievable between its endpoints. Even though in this thesis, we only prove the above results for 90°-chains, we believe that the results hold for α-chains for abitrary α. It is likely that the polynomial time bound only holds for α-chains, and that, in its full generality, 3D max span is NP-hard. This is because the planar sections are no longer guaranteed to be in the *trans*-configuration, so one must resort to computing the max flat spans of the planar subchains (which can become arbitrarily large if alignment of subsubchains is not possible), which Soss proved was NP-hard [Sos01].

Finally, it was suggested to us by Professor Ruth Haas that our results may extend to arbitrary dimensions. This remains to be proved.

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