On the Maximum Span of Fixed-Angle Chains

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Abstract

Soss proved that it is NP-hard to find the maximum flat span of a fixed-angle polygonal chain: the largest distance achievable between the endpoints in a planar embedding. These fixed-angle chains can serve as models of protein backbones. The corresponding problem in 3D is open. We show that two special cases of particular relevance to the protein model are solvable in polynomial time: when all link lengths are equal, and all angles are equal, the maximum 3D span is achieved in a flat configuration and can be computed in constant time. When all angles are equal (but the link lengths arbitrary), the maximum 3D span is in general nonplanar but can be found in polynomial time.

1 Introduction

Polygonal chains with fixed joint angles, permitting "dihedral" spinning about each edge, have been used to model the geometry of protein backbones [ST00] [DLO06]. 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 maxspan problem, and we do the same. We make progress on the 3D maxspan problem by focusing on restricted classes of chains, which are incidentally among the most relevant under the protein model.

Let a polygonal chain C have vertices $(v_0, v_1, \ldots, v_n)$. The fixed joint angle is $\alpha_i = \angle v_{i-1} v_i v_{i+1}$. Define an α-*chain* as one all of whose joint angles are the same angle α. Protein backbones can be crudely modeled as α-chains, with α obtuse, roughly in $[109°, 122°]$. De-

fine a *unit* chain[1] as one all of whose link lengths are 1. Again roughly, protein backbones have equal-length links, because the bonds along the backbone lie in the range [1.33Å,1.52Å].

We can summarize Soss's investigation in the first two lines of Table 1, and our results in the last three lines. 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 $\tau = \pi - \alpha$ 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 maxspan configuration might be nonplanar. For α-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 α-chains to be found via a dynamic programming algorithm in $O(n^3)$ time.

Chain	dim	angles	lengths	complexity
fixed-angle	2	arbitrary	arbitrary	NP-hard
chains	3	arbitrary	arbitrary	?
unit α-chains	3	$= \alpha$	1	$O(1)$
α-chains	2	$= \alpha$	arbitrary	$O(n)$
	3	$= \alpha$	arbitrary	$O(n^3)$

Table 1: Maxspan Computational Complexities.

2 Basic Lemmas

We start with two lemmas which hold for arbitrary joint angles and arbitrary link lengths. Proofs not included in this abstract may be found in [Ben06].

Lemma 1 (3-Chain Lemma) *The maximum span of any fixed-angle 3-chain is achieved in a planar configuration.*

See Fig. 1.
A near-immediate corollary is:

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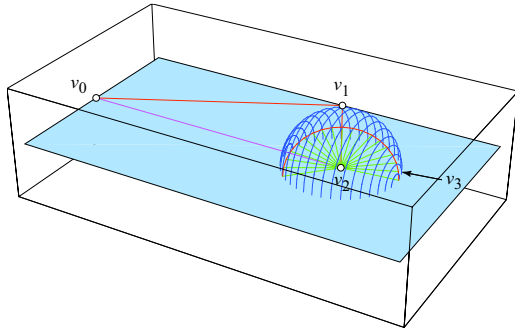
[1]The terminology is from [Poo05].

Figure 1: The maximum span of a fixed-angle 3-chain is achieved in a flat configuration. The rim of the cone is the locus of possible locations of v_3. The cone ribs specify all possible locations of edge v_2v_3, which rides along a cone whose axis is v_1v_2. The blue rings are the level sets for $\beta = \angle v_0v_2v_3$. The maxspan is achieved when β is maximized with v_3 in the plane of $\{v_0, v_1, v_2\}$.

Lemma 2 (4-Vertex Lemma) *Let* $(v_0, v_1, \ldots, v_k)$ *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.*
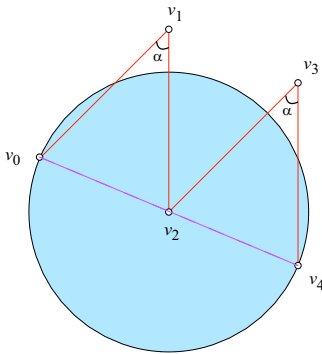

Figure 2: The maximal configuration of a unit, α- 4-chain. The maxspan is $2\,|v_0v_2|$.

3   Unit Chains

Now we specialize to unit α-chains. Our first lemma will serve as the base case in an induction proof to follow.

Lemma 3 *The maximum span of a unit α-chain of 4 links, is achieved in a planar configuration.*

See Fig. 2. This lemma is false without either the unit-length or the same-angle assumptions. Fig. 3 shows an example establishing the latter claim.

We now turn to unit α-chains of an arbitrary number of links. Our main result here is:

Theorem 4 *The maximum span of any unit α-chain is achieved in the planar trans-configuration.*
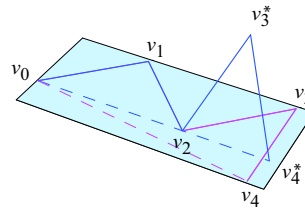

Figure 3: A unit, fixed-angle chain with non-equal joint angles, whose maximal configuration is nonplanar. The nonplanar span is ≈ 2.18, while the flat span is ≈ 2.17.

See Fig. 4. Clearly, this theorem permits computation of the maxspan under these circumstances in constant time, as in Table 1. The induction argument is different
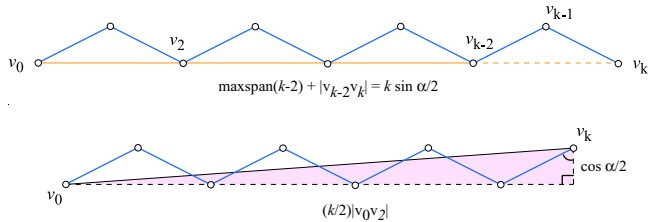

Figure 4: The maximal configurations of a unit α-chains.

for an even and odd number of links. For even n, we remove two links, apply induction, and the result follows easily. The argument for odd links is more delicate. The key construction is displayed in Fig. 5. We prove that maxspan is achieved in this figure when $v_0 = v^*$.

4   Planar Trans-Configuration

Although Theorem 4 fails without the unit-length assumption, if we restrict an α-chain to the plane, then its max flat span is still the trans-configuration:

Theorem 5 *If C is an α-chain (in general with different link lengths), then the maximum flat span of C is realized in the trans-configuration.*
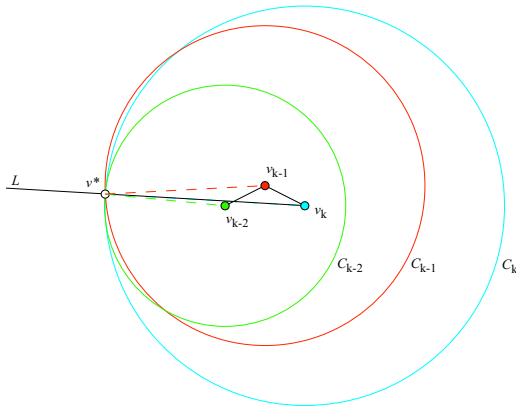
Figure 5: C_{k-2} is a circle of radius maxspan $|k-2| =$ transspan $|k-2|$ centered at v_{k-2}, C_{k-1} is a circle of radius maxspan $|k-1| =$ transspan $|k-1|$ centered at v_{k-1}, and C_k is a circle of radius transspan $|k|$ centered at v_k. The circles C_{k-2}, C_{k-1}, and C_k intersect at the common point v^*.

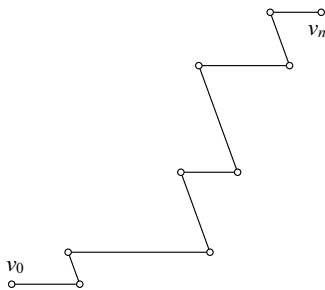See Fig. 6 for an example. This theorem permits com-

Figure 6: Planar trans-configuration of an α-chain with with acute α.

putation of the max flat span of an α-chain in $O(n)$ time, as in Table 1.

5 5-Chain Analysis

The structure Theorem 6 below relies on a close analysis of 5-chains, to which sections of an n-chain may be reduced. We henceforth specialize all figures to $\alpha = 90°$, the easiest angle to comprehend. Fig. 7 shows a 5-chain in maxspan configuration. By Lemma 2, we know v_5 must lie in the plane of $\{v_0, v_1, v_2\}$. We analyze how the reachability region of v_5, as the end of a 3-link chain from origin v_2, intersects the xy-plane. This reachability region is depicted in Fig. 8, and its intersection with the plane is shown in Fig. 9.

6 Structure Theorem

We wrote code to find the maximum span configurations of n-link chains empirically by gradient ascent. Typical
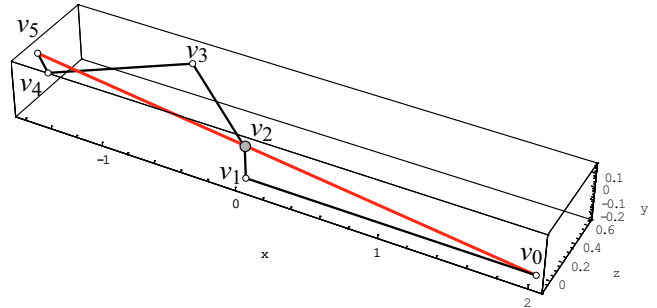

Figure 7: The maximum span of a 90° 5-chain with link lengths $(2, \frac{1}{4}, 1, 1, \frac{1}{4})$. The last three links correspond to Figs. 8. and 9.
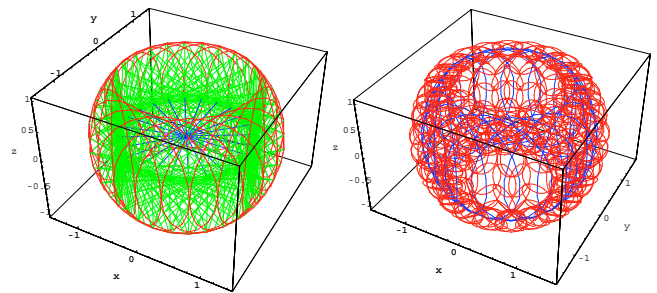

Figure 8: A 2-chain torus (left) generated by link lengths $(1, 1)$, and a 3-chain torus (right) generated by lengths $(1, 1, \frac{1}{4})$, both for $\alpha = 90°$. The right figure corresponds to the quadrilaterals in Fig. 9.
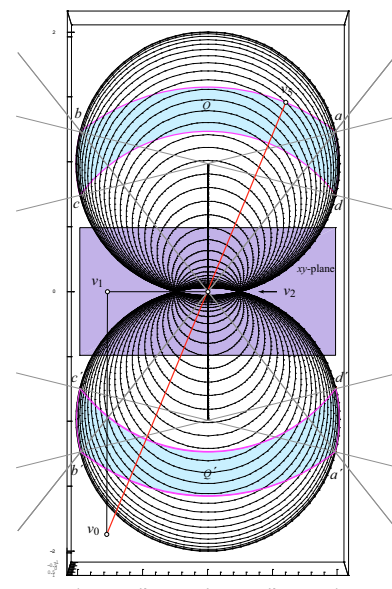

Figure 9: The region corresponding to configurations which place v_5 in the plane is a quadrilateral (blue region). The lengths of the $(v_2 - v_5)$ 3-chain are $(1, 1, \frac{1}{4})$.
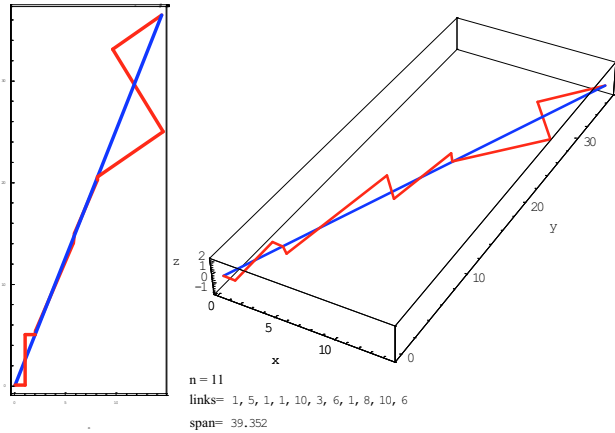
Figure 10: Two views of an 11-chain: 3+5+3 subchains.

output is shown in Fig. 10. It was these empirical results that suggested our main structural theorem:

Theorem 6 (Structure Theorem) *The maxspan configuration for an α-chain is either:*

1. *planar: in trans-configuration*

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

   (a) *is in maxspan trans-configuration; and*
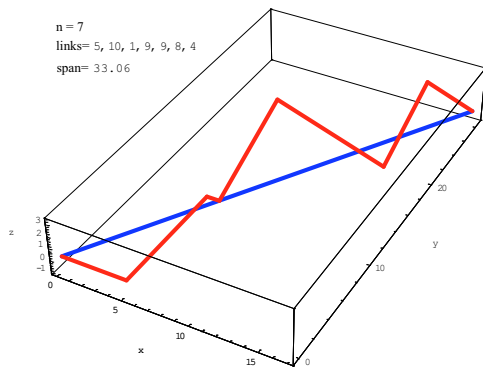
   (b) *whose spans align collinearly.*

Figure 11: A 7-chain composed of a maxspan 3-chain aligned with a maxspan 4-chain.

7 Dynamic Programming Algorithm

In general, hardness of computing the maximum span in 3D is not known. However, the structure theorem permits it to be computed in $O(n^3)$ time via a dynamic

programming algorithm for α-chains, the last line of Table 1. The computation for the example in Fig. 11 is shown in Table 7.

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.

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