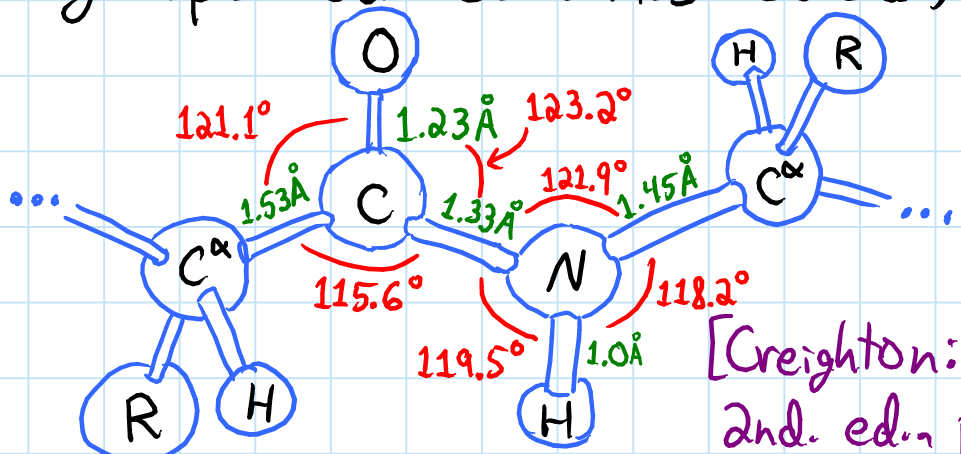
6.885	Lecture 16	Nov. 5, 2007

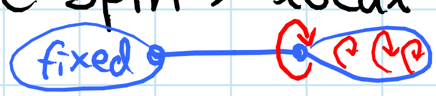
Fixed-angle linkages: fix angles between incident bars

- roughly the mechanics of a protein (of L15)
- in fact, roughly fixed-angle tree
- protein backbone is roughly fixed-angle chain (usually open but sometimes closed)



[Creighton: PROTEINS, 2nd. ed., p. 5]

- usually focus on backbone, ignoring amino-acid "side chains" ~ reasonable approximation
- basic move: edge spin / local dihedral motion:



Major problems in fixed-angle linkages (esp. chains)

1. (un)locked = motion between any two states
2. flattening = motion to flat state
3. flat-state connectivity = motions between flat states
4. span = max/min distance between endpoints

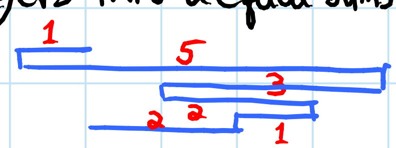
Locked proteins:

- locked universal-joint chains are locked fixed-angle too
  - even simpler, 4-link "crossed-legs":

- existence of locked chains suggests config. space is hard to navigate ~ but nature does it well
- Conjecture: additional constraints in nature prevent existence of locked chains
  - bond lengths all roughly equal (1-1.53Å)
  - bond angles all obtuse & roughly equal (115.6-123.2°)
  - $\boxed{\text{OPEN}}$: is there a locked fixed-angle chain that's equilateral, equiangular, & obtuse
    - crossed legs satisfies all but obtuse
  - proteins produced sequentially by ribosome [L18]

Flattening: weakly NP-hard [Soss & Toussaint 2000]

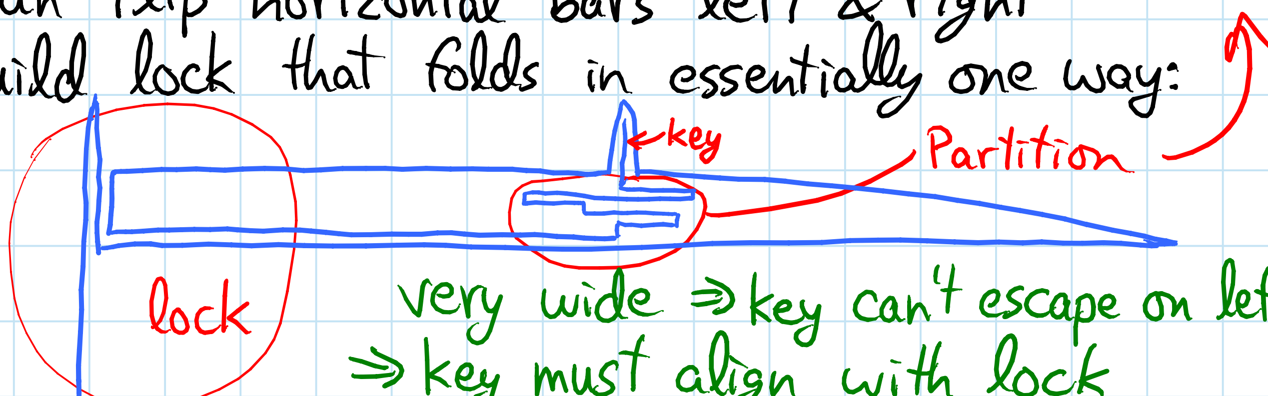
- reduction from Partition: divide n integers into 2 equal sums
- horizontal bars for integers



- vertical bars in between, length $< \frac{1}{n}$

⇒ can flip horizontal bars left & right

- build lock that folds in essentially one way:

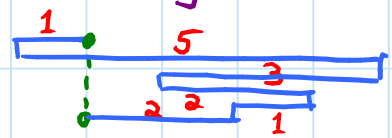


very wide ⇒ key can't escape on left
⇒ key must align with lock

$\boxed{\text{OPEN}}$: pseudopolynomial-time algorithm?

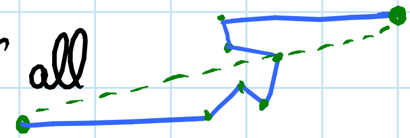
<u>Span</u> of chain configuration = distance between endpoints
- distribution of span over configuration space heavily studied in e.g. polymer physics [>20 papers]

<u>Flat min span</u>: weakly NP-hard [Soss 2001]
- first part of previous reduction:



- min span $< 1 \iff$ <u>horiz. aligned</u>

<u>Flat max span</u>: weakly NP-hard [Soss 2001]
- another reduction from Partition
- each turn angle = integer/sum of all



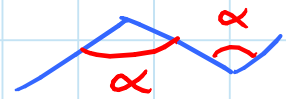
- end bars very long; rest short
- max span when long bars parallel & point away
  i.e. $\Sigma \pm$ turn angles $= \emptyset$

$\boxed{\text{OPEN}}$: pseudopoly. alg. for flat min/max. span?
$\boxed{\text{OPEN}}$: complexity of 3D min/max.?

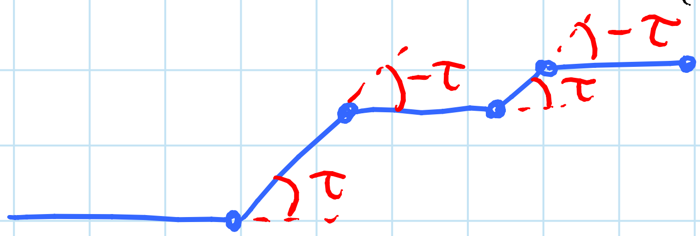
<u>Equiangular case</u>: max span polynomial, even in 3D!
[Benbernou & O'Rourke 2006]
- also equilateral $\Rightarrow$ constant time
- in general: nice structure theorem
  & $O(n^3)$ time
  ↳ rest of lecture

Nadia:

<u>α-chain</u> = fixed-angle chain where every angle $= \alpha$



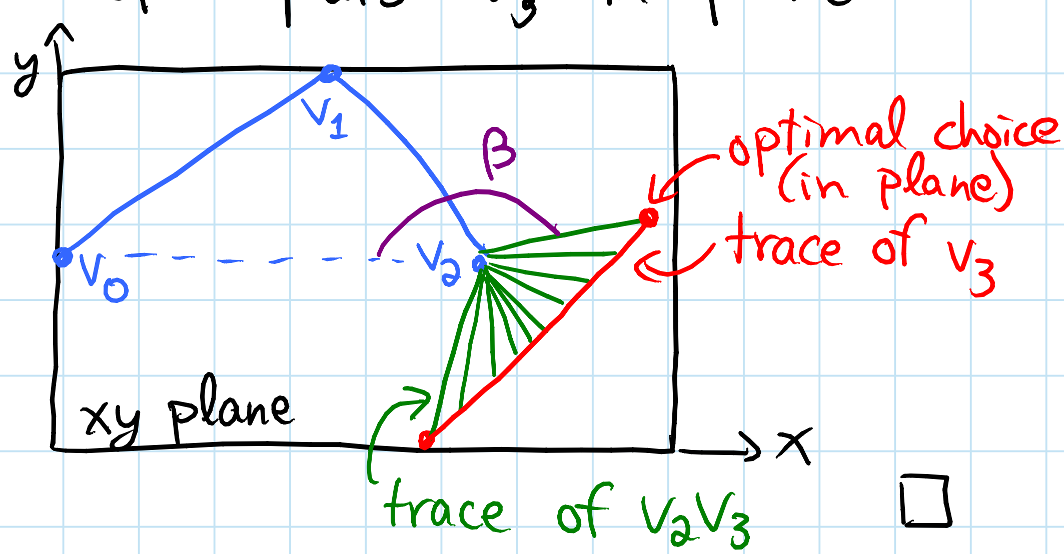
<u>Trans configuration</u> = turn angles alternate between $\pm \tau$



(only meaningful for α-chains)

<u>3-chain lemma</u>: max span of 3-bar fixed-angle chain is achieved by planar trans configuration

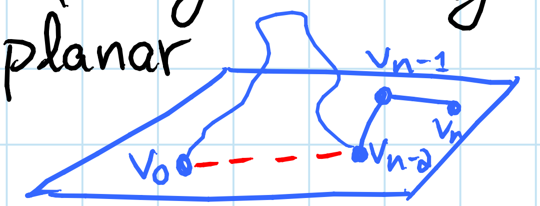
<u>Proof</u>: β = angle between $v_0 v_2$ & $v_2 v_3$
assume v_0, v_1, v_2 in xy plane
assume v_0, v_2 on x axis
max span puts v_3 in plane



$\square$

Nadia: (cont'd)

4-vertex lemma: in any max span configuration of k-link chain $v_0, v_1, \dots, v_k$, v_0, v_1, v_2, v_k are coplanar, & symmetrically $v_0, v_{k-2}, v_{k-1}, v_k$ are coplanar



Proof: we'll show latter (enough by symmetry)
make virtual link $v_0 \to v_{k-2}$
get induced 3-link chain $v_0, v_{k-2}, v_{k-1}, v_k$
max span of orig. = max span of this
3-chain lemma ⇒ planar
⇒ $v_0, v_{k-2}, v_{k-1}, v_k$ are coplanar □

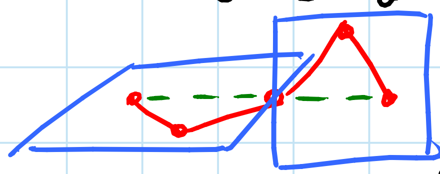
Equilateral α-chain achieves max span in planar trans configuration
⇒ can compute max span in $O(1)$ time
(not covering proof)

Max flat span of α-chain is trans config
⇒ can compute in $O(n)$ time
(not covering proof)

Nadia: (cont'd)

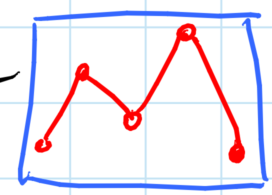
4-link structure: max span of 4-link fixed-angle chain is achieved in one of two ways:

1. spans of (v_0, v_1, v_2) & (v_2, v_3, v_4) align



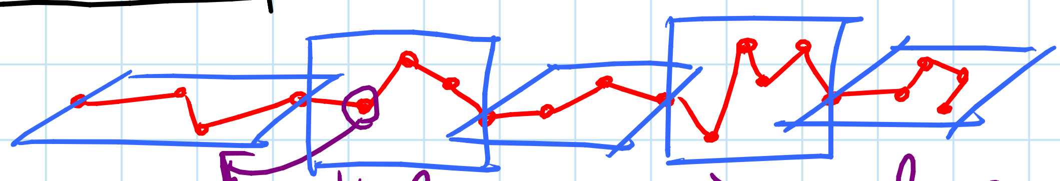
i.e. v_0, v_2, v_4 collinear

2. entire configuration is planar



(not covering proof)

Partition into planar sections:



Structure theorem: max span of n-link fixed-angle chain can be partitioned into planar sections each

(a) aligning spans collinearly with its neighboring sections

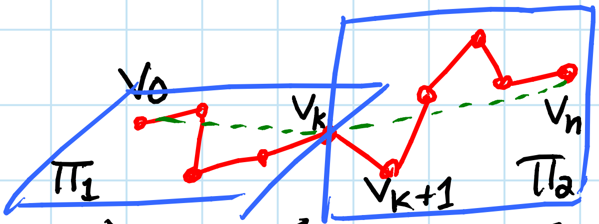
(b) in its own max span configuration

Nadia: (Cont'd)

Proof sketch of ⓐ:
by induction on $m = \#$ planar sections

Base case: $m=1$ trivial

Base case: $m=2$



$C = C_1 \cup C_2$

- >1 link in C_2 by 4-vertex lemma
- suppose for contradiction that v_0, v_k, v_n are not collinear
- virtual chains $C_1' = (v_0, v_{k-1}, v_k)$ & $C_2' = (v_k, v_{k+1}, v_n)$
  - same spans & same angle at v_k
- apply 4-link structure theorem to $C' = C_1' \cup C_2'$

$\Rightarrow$ either planar ~ but then $\Pi_1 = \Pi_2$
or spans of C_1' & C_2' align
i.e. v_0, v_k, v_n collinear

$\Rightarrow$ contradiction

General case: similar but messier $\square$

Nadia: (cont'd)

Dynamic program for max span of α-chain

- exploit planar trans config. in each planar region
- subproblem = subchain $(v_i, v_{i+1}, \dots, v_j)$ ← $O(n^2)$
- guess partition point v_k between two planes
- look at subproblems $(v_i, \dots, v_k)$ & $(v_k, \dots, v_j)$
- check whether max spans of these two recursive subproblems can align:
  - attach at v_k so that collinear with v_0 & v_n
  - unlikely to get right angle at v_k
  - spin plane of latter chain
  - if at some point angle at v_k is correct then this *must* be max span
- else must be flat trans configuration
  only place we use that it's α-chain!

$\Rightarrow O(n^3)$ time

Optimization to $O(n^2)$ time:

- subproblem = subchain $(v_i, \dots, v_n)$ $\Rightarrow O(n)$
- guess *first* partition point v_k
- $\Rightarrow (v_i, \dots, v_k)$ guaranteed planar
- so just recurse on $(v_k, \dots, v_n)$