Did you know that Multiple Alignment is NP-hard?

Isaac Elias

Royal Institute of Technology
Sweden

Results

- Multiple Alignment with SP-score
- Star Alignment
- Tree Alignment (with given phylogeny)

are NP-hard under all metrics!

Pairwise Alignment

Mutations: substitutions, insertions, and deletions.

Input: Two related strings s_1 and s_2.

Output: The least number of mutations needed to $s_1 \rightarrow s_2$.

$$
\begin{array}{llllllll}
s_1 = & & a & a & g & a & c & t \\
s_2 = & & a & g & t & g & c & t
\end{array}
$$

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$2 \times l$ matrix A

$$\begin{array}{lccccccc} s_1 = & \text{a} & \text{a} & \text{g} & \text{a} & - & \text{c} & \text{t} \\ s_2 = & - & \text{a} & \text{g} & \text{t} & \text{g} & \text{c} & \text{t} \end{array}$$

$\mathtt{d}_A(s_1, s_2) = 3$ mutations

Metric symbol distance

Unit metric - binary alphabet
(the edit distance)

Σ	$\mathbf{0}$	$\mathbf{1}$	$-$
$\mathbf{0}$	0	1	1
$\mathbf{1}$	1	0	1
$-$	1	1	0

Metric symbol distance

Unit metric - binary alphabet
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Σ	**0**	**1**	$-$
0	0	1	1.5
1	1	0	1.5
$-$	1.5	1.5	0

Insertions and deletions occur less frequently!

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Unit metric - binary alphabet
(the edit distance)

Σ	**0**	**1**	$-$
0	0	1	1
1	1	0	1
$-$	1	1	0

Insertions and deletions occur less frequently!

General metric - α, β, γ have metric properties
(identity, symmetry, triangle ineq.)

Σ	**0**	**1**	$-$
0	0	α	β
1	α	0	γ
$-$	β	γ	0

Multiple Alignment

When sequence similarity is low pairwise alignment may fail to find similarities.

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Output: $k \times l$ matrix A.

a	a	g	a	-	c	t
-	-	g	a	g	c	t
a	c	g	a	g	c	-
a	-	g	t	g	c	t

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a	c	g	a	g	c	-
a	-	g	t	g	c	t

How do we score columns?

Sum of Pairs score (SP-score)

Let the cost be the sum of costs for all pairs of rows:

$$\sum_{i=1}^{k}\sum_{j=i}^{k}\mathtt{d}_A(s_i,s_j),$$

where $\mathtt{d}_A(s_i,s_j)$ is the pairwise distance between the rows containing strings s_i and s_j.

Earlier NP results

- Wang and Jiang '94 - Non-metric
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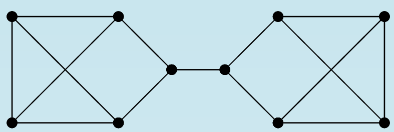
Here: All binary or larger alphabets under all metrics!

Independent R3 Set

Independent set in three regular graphs, i.e. all vertices have degree 3, is NP-hard.

Input: A three regular graph $G = (V, E)$ and a integer c.

Output: "Yes" if there is an independent set $V' \subseteq V$ of size $\geq c$, otherwise "No".



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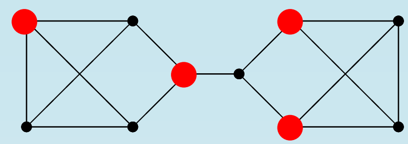

Reduction

Independent R3 Set		**SP-score**
$G = (V, E)$	$\longrightarrow$	Set of strings
c		K
set of size $\geq c$		matrix of cost $\leq K$
V'	$\longleftrightarrow$	A

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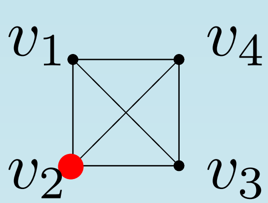


	v_1		v_2		v_3		v_4	
	1	0...0...	1	0...0...	1	0...0...	1	
	⋮	⋮ ⋮	⋮	⋮ ⋮	⋮	⋮ ⋮	⋮	
	1	0...0...	1	0...0...	1	0...0...	1	
			1					
			⋮					
			1					
	0	0...10...	1	0...0...	0	0...0...	0	0...
0...	1	0...0...	0	0...10...	0	0...0...	0	
	0	0...10...	0	0...0...	0	0...0...	1	0...
0...	0	0...0...	1	0...10...	0	0...0...	0	
0...	0	0...0...	1	0...0...	0	0...10...	0	
0...	0	0...0...	0	0...0...	1	0...10...	0	

Gadgetering

1. Each vertex is represented by a column (n vertex columns).

2. c vertex columns are picked.

3. Each edge is represented by an edge string.

	v_1		v_2	$\ldots$	v_i	$\ldots$	v_n	
	1	0...0...	1	$\ldots$	1	$\ldots$	1	
	$\vdots$	$\vdots$ $\vdots$	$\vdots$	$\vdots$ $\vdots$	$\vdots$	$\ldots$	$\vdots$	
	1	0...0...	1	$\ldots$	1	$\ldots$	1	
			1		1			
			$\vdots$		$\vdots$			
			1		1			
	0	0...10...	1	0...0...	0	0...0...	0	0...
0...	1	0...0...	0	0...10...	0	0...0...	0	
	0	0...10...	0	0...0...	0	0...0...	1	0...
0...	0	0...0...	1	0...10...	0	0...0...	0	
0...	0	0...0...	1	0...0...	0	0...10...	0	
0...	0	0...0...	0	0...0...	1	0...10...	0	

Template strings $\to$ Vertex columns

We add **very** many template strings:

$$T = (10^b)^{n-1}1$$

	v_1		v_2	$\ldots$	v_i	$\ldots$	v_n	
	1	$0 \ldots 0 \ldots$	1	$\ldots$	1	$\ldots$	1	
	$\vdots$	$\vdots \quad \vdots$	$\vdots$	$\vdots \quad \vdots$	$\vdots$	$\ldots$	$\vdots$	
	1	$0 \ldots 0 \ldots$	1	$\ldots$	1	$\ldots$	1	

Fact: Identical strings are aligned identically in an optimal alignment.

Pick strings $\rightarrow V' \subseteq V$

We add **very** many pick strings: $P = 1^c$.

	v_1		v_2	$\dots$	v_i	$\dots$	v_n	
	1	$0 \dots 0 \dots$	1	$\dots$	1	$\dots$	1	
	$\vdots$	$\vdots \quad \vdots$	$\vdots$	$\vdots \quad \vdots$	$\vdots$	$\dots$	$\vdots$	
	1	$0 \dots 0 \dots$	1	$\dots$	1	$\dots$	1	
			1		1			
			$\vdots$		$\vdots$			
			1		1			

Fact: c vertex columns are picked since this is the alignment with least missmatches.

Edge strings

Property: If there is an edge (v_i, v_j) then both v_i and v_j can not be part of the independent set.

$$E_{ij} = 0^s(00^b)^{i-1}10^{b-s}(00^b)^{j-i-1}10^b(00^b)^{n-j-1}00^s$$

		v_1		v_i	$\ldots \quad \ldots$	v_j	$\ldots$	v_n	
		1	0. . . 0. . .	1	$\ldots \quad \ldots$	1	$\ldots$	1	
		$\vdots$	$\vdots \quad \vdots$	$\vdots$	$\ldots \quad \ldots$	$\vdots$	$\ldots$	$\vdots$	
		1	0. . . 0. . .	1	$\ldots \quad \ldots$	1	$\ldots$	1	
good	0^s	0	0. . . 0. . .	1	0. . . $1\ 0^{s-1}$	0	0. . . 0. . .	0	
good		0	0. . . 0. . .	0	$0^{s-1}\ 1$ 0. . .	1	0. . . 0. . .	0	0^s
bad	0^s	0	0. . . 0. . .	1	$-^s$ 0. . .	1	0. . . 0. . .	0	0^s

Independent set $\geq c \Leftrightarrow$ Alignment $\leq K$

$$K = (n-c)\gamma b^2 + b(n-1)\beta b^2 + (s\beta + n\alpha)bm + \Big(c\alpha + (s + b(n - 1) + n - c - 2)\beta + 2\gamma\Big)bm - 3cb(\alpha + \gamma - \beta) + (s\beta + 2\alpha)m^2$$

Independent set $\geq c \Leftrightarrow$ Alignment $\leq K$

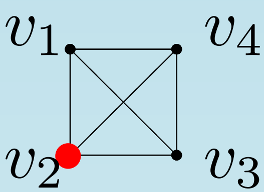
1. Remember three regular graph. So there are atmost three ones in each vertex column.

2. If a column with only two ones is picked then there is a missmatch extra for each pick string ($\Rightarrow$ score $> K$).

Example

1. Atmost three ones in each vertex column.

2. Pick strings pick columns with most ones.



		v_1		v_2		v_3		v_4	
		1	0. . . 0. . .	1	0. . . 0. . .	1	0. . . 0. . .	1	
		⋮	⋮ ⋮	⋮	⋮ ⋮	⋮	⋮ ⋮	⋮	
		1	0. . . 0. . .	1	0. . . 0. . .	1	0. . . 0. . .	1	
				1					
				⋮					
				1					
E_{12}		**0**	**0. . . 10. . .**	**1**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	**0. . .**
E_{13}	0. . .	1	0. . . 0. . .	0	0. . . 10. . .	0	0. . . 0. . .	0	
E_{14}		0	0. . . 10. . .	0	0. . . 0. . .	0	0. . . 0. . .	1	0. . .
E_{23}	0. . .	0	0. . . 0. . .	1	0. . . 10. . .	0	0. . . 0. . .	0	
E_{24}	**0. . .**	**0**	**0. . . 0. . .**	**1**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	
E_{34}	0. . .	0	0. . . 0. . .	0	0. . . 0. . .	1	0. . . 10. . .	0	

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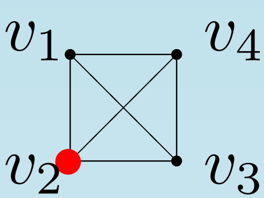

		v_1		v_2		v_3		v_4	
		1 ⋮ 1	0. . . 0. . . ⋮ ⋮ 0. . . 0. . .	1 ⋮ 1	0. . . 0. . . ⋮ ⋮ 0. . . 0. . .	1 ⋮ 1	0. . . 0. . . ⋮ ⋮ 0. . . 0. . .	1 ⋮ 1	
				1 ⋮ 1					
E_{12}	**0. . .**	**1**	**0. . . 10. . .**	**0**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	
E_{13}	0. . .	1	0. . . 0. . .	0	0. . . 10. . .	0	0. . . 0. . .	0	
E_{14}		0	0. . . 10. . .	0	0. . . 0. . .	0	0. . . 0. . .	1	0. . .
E_{23}	0. . .	0	0. . . 0. . .	1	0. . . 10. . .	0	0. . . 0. . .	0	
E_{24}	**0. . .**	**0**	**0. . . 0. . .**	**1**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	
E_{34}	0. . .	0	0. . . 0. . .	0	0. . . 0. . .	1	0. . . 10. . .	0	

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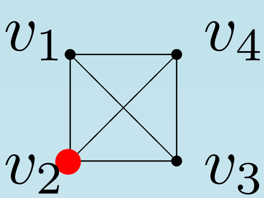

		v_1 1 ⋮ 1	0. . . 0. . . ⋮ ⋮ 0. . . 0. . .	v_2 1 ⋮ 1	0. . . 0. . . ⋮ ⋮ 0. . . 0. . .	v_3 1 ⋮ 1	0. . . 0. . . ⋮ ⋮ 0. . . 0. . .	v_4 1 ⋮ 1	
				1 ⋮ 1					
E_{12}	**0. . .**	**1**	**0. . . 10. . .**	**0**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	
E_{13}	0. . .	1	0. . . 0. . .	0	0. . . 10. . .	0	0. . . 0. . .	0	
E_{14}		0	0. . . 10. . .	0	0. . . 0. . .	0	0. . . 0. . .	1	0. . .
E_{23}	0. . .	0	0. . . 0. . .	1	0. . . 10. . .	0	0. . . 0. . .	0	
E_{24}		**0**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**1**	**0. . .**
E_{34}	0. . .	0	0. . . 0. . .	0	0. . . 0. . .	1	0. . . 10. . .	0	

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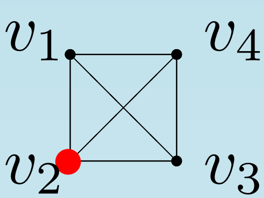

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		1	0. . . 0. . .	1	0. . . 0. . .	1	0. . . 0. . .	1	
		⋮	⋮ ⋮	⋮	⋮ ⋮	⋮	⋮ ⋮	⋮	
		1	0. . . 0. . .	1	0. . . 0. . .	1	0. . . 0. . .	1	
		1							
		⋮							
		1							
E_{12}	**0. . .**	**1**	**0. . . 10. . .**	**0**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	
E_{13}	0. . .	1	0. . . 0. . .	0	0. . . 10. . .	0	0. . . 0. . .	0	
E_{14}		0	0. . . 10. . .	0	0. . . 0. . .	0	0. . . 0. . .	1	0. . .
E_{23}	0. . .	0	0. . . 0. . .	1	0. . . 10. . .	0	0. . . 0. . .	0	
E_{24}		**0**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**0**	**0. . . 0. . .**	**1**	**0. . .**
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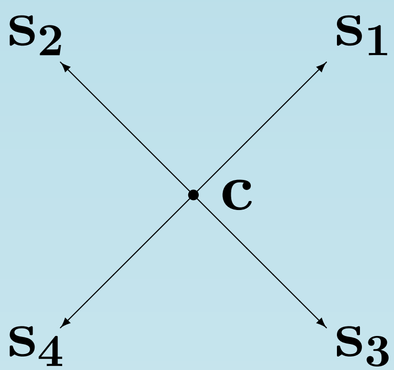
Star Alignment

SP-score not a good model of evolution.



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$$\sum_i \mathtt{d}(c, s_i)$$

$\mathbf{s_2}$ $\mathbf{s_1}$

?

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Symbol distance metric $\Longrightarrow$ Pairwise alignment distance metric

Star Alignment is a special case of **Steiner Star** in a metric space.

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Vertex Cover		**Star Alignment**
$G = (V, E)$	$\longrightarrow$	Set of strings
minimum cover		minimum string
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$G = (V, E)$	$\longrightarrow$	Set of strings
minimum cover		minimum string
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$$
\begin{array}{cc|c|c|c|c|c|c|c|c}
 & & \mathbf{v_1} & & \mathbf{v_2} & & \mathbf{v_3} & \ldots & \mathbf{v_n} & \\
\hline
\mathbf{C} \quad = & \ldots & ? & \ldots & ? & \ldots & ? & \ldots & ? & \ldots \\
\hline
\end{array}
$$

Reduction

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$G = (V, E)$	$\longrightarrow$	Set of strings
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$$\mathbf{C_V} = \begin{array}{c|c|c|c|c|c|c|c|c} & \mathbf{v_1} & & \mathbf{v_2} & & \mathbf{v_3} & \mathbf{\ldots} & \mathbf{v_n} & \\ \hline \ldots & \mathbf{1} & \ldots & \mathbf{1} & \ldots & \mathbf{1} & \ldots & \mathbf{1} & \ldots \\ \hline \end{array}$$

C_V - Only **1's**.

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		$\mathbf{v_1}$		$\mathbf{v_2}$		$\mathbf{v_3}$	$\dots$	$\mathbf{v_n}$	
$\mathbf{C_\emptyset} =$	$\dots$	$\mathbf{0}$	$\dots$	$\mathbf{0}$	$\dots$	$\mathbf{0}$	$\dots$	$\mathbf{0}$	$\dots$

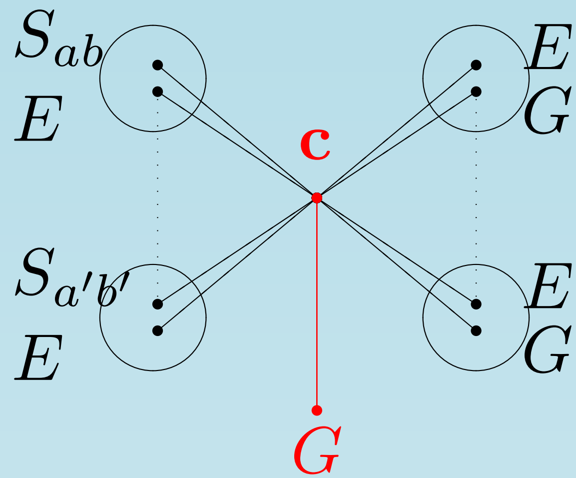
C_V - Only **1's**. $C_\emptyset$ - Only **0's**.

Construction Idea

$(E, G) \quad \longrightarrow \quad c = DDCDD$

$(E, S_{ab}) \quad \longrightarrow \quad c =$ vertex cover

$G \quad \longrightarrow \quad$ minimum cover



String minimizing $\sum_i \mathtt{d}(c, s_i) \leftrightarrow$ minimum cover

Canonical Structure

$$E = DDC_V DD \qquad G = DDC_\emptyset DD$$

Differ only in the vertex positions.

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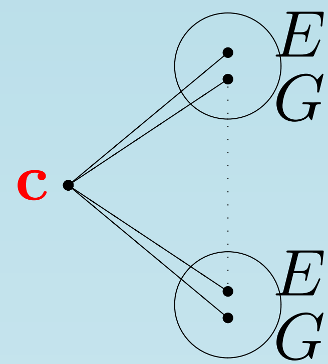

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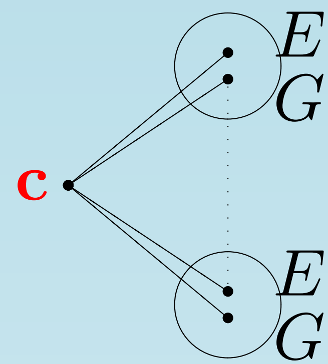

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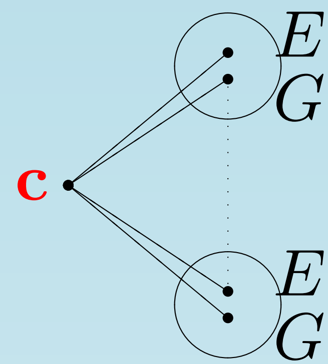

$$\Rightarrow \mathbf{c} = \mathbf{DDCDD}$$

String $\longrightarrow$ Cover

Edge (v_a, v_b) add two strings

$$E = DDC_V DD \qquad\qquad S_{ab} = C_a D C_b$$

$$\mathbf{C_a} = \begin{array}{c|c|c|c|c|c|c|c|c} & \mathbf{v_1} & \ldots & \mathbf{v_a} & \ldots & \mathbf{v_b} & \ldots & \mathbf{v_n} & \\ \hline \ldots & \mathbf{0} & \ldots & \mathbf{1} & \ldots & \mathbf{0} & \ldots & \mathbf{0} & \ldots \\ \hline \end{array}$$

String $\longrightarrow$ Cover

Edge (v_a, v_b) add two strings

$$E = DDC_V DD \qquad\qquad S_{ab} = C_a D C_b$$

$$\mathbf{C_b} \;=\; \begin{array}{c|c|c|c|c|c|c|c|c} & \mathbf{v_1} & \ldots & \mathbf{v_a} & \ldots & \mathbf{v_b} & \ldots & \mathbf{v_n} & \\ \hline \ldots & \mathbf{0} & \ldots & \mathbf{0} & \ldots & \mathbf{1} & \ldots & \mathbf{0} & \ldots \\ \hline \end{array}$$

String $\longrightarrow$ Cover

Edge (v_a, v_b) add two strings

$$E = DDC_V DD \qquad\qquad S_{ab} = C_a D C_b$$

E votes **1** in all vertex positions.

String $\longrightarrow$ Cover

Edge (v_a, v_b) add two strings

$$E = DDC_V DD \qquad S_{ab} = C_a D C_b$$

E votes **1** in all vertex positions.
S_{ab} votes **0** in all except vertex position a or b.

$$\begin{array}{cc|c|cc} D & D & C & D & D \\ C_a & D & C_b & & \\ & & C_a & D & C_b \end{array}$$

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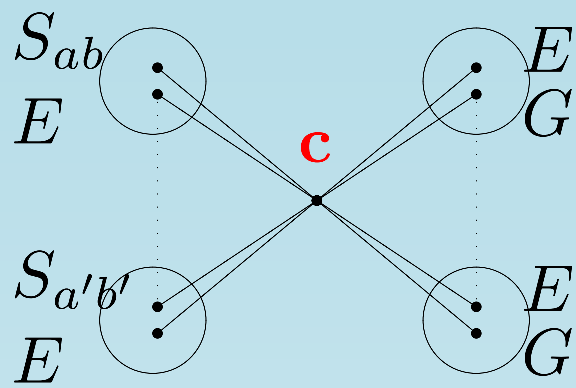
Either vertex v_a or vertex v_b is part of the cover.

Minimal String $\leftrightarrow$ Minimum Cover

$$(E, G) \quad \rightarrow \quad c = DDCDD$$

$$(E, S_{ab}) \quad \rightarrow \quad c = \text{vertex cover}$$



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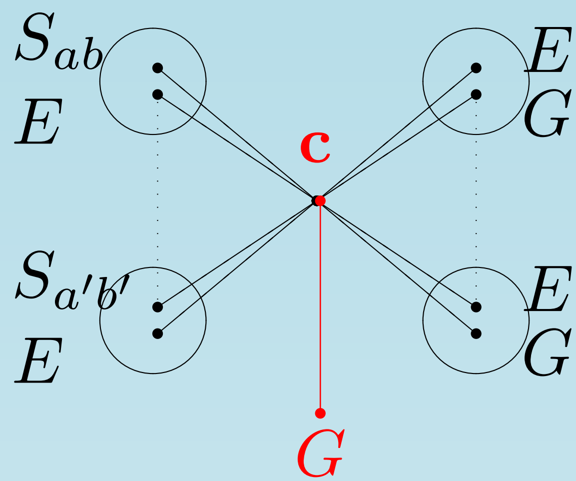

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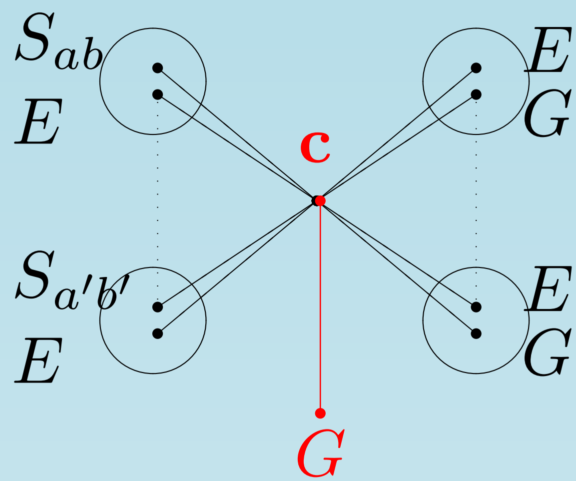

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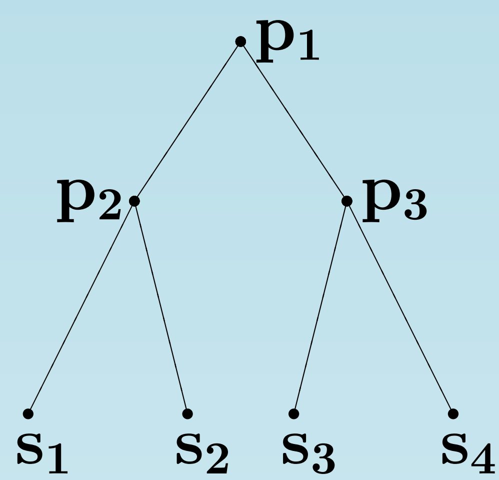
String minimizing $\sum_i \mathrm{d}(c, s_i) \leftrightarrow$ minimum cover

Tree Alignment (given phylogeny)

STAR ALIGNMENT not a good model of evolution.



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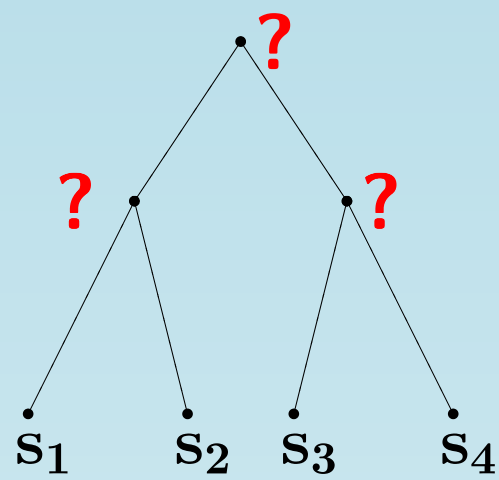
Input: k strings $s_1 \ldots s_k$
phylogeny T
Output: strings $p_1 \ldots p_{k-1}$

$$\min \sum_{(a,b) \in \mathtt{E}(T)} \mathtt{d}(a, b)$$



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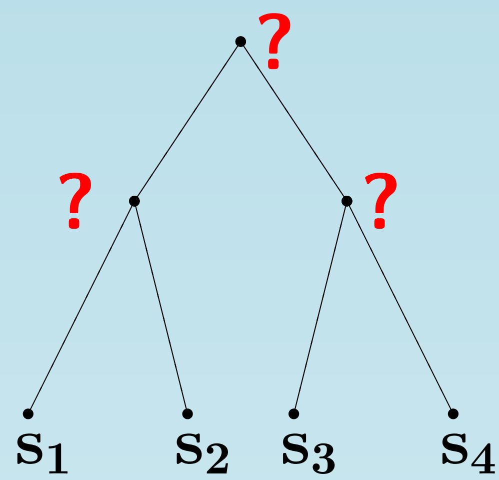
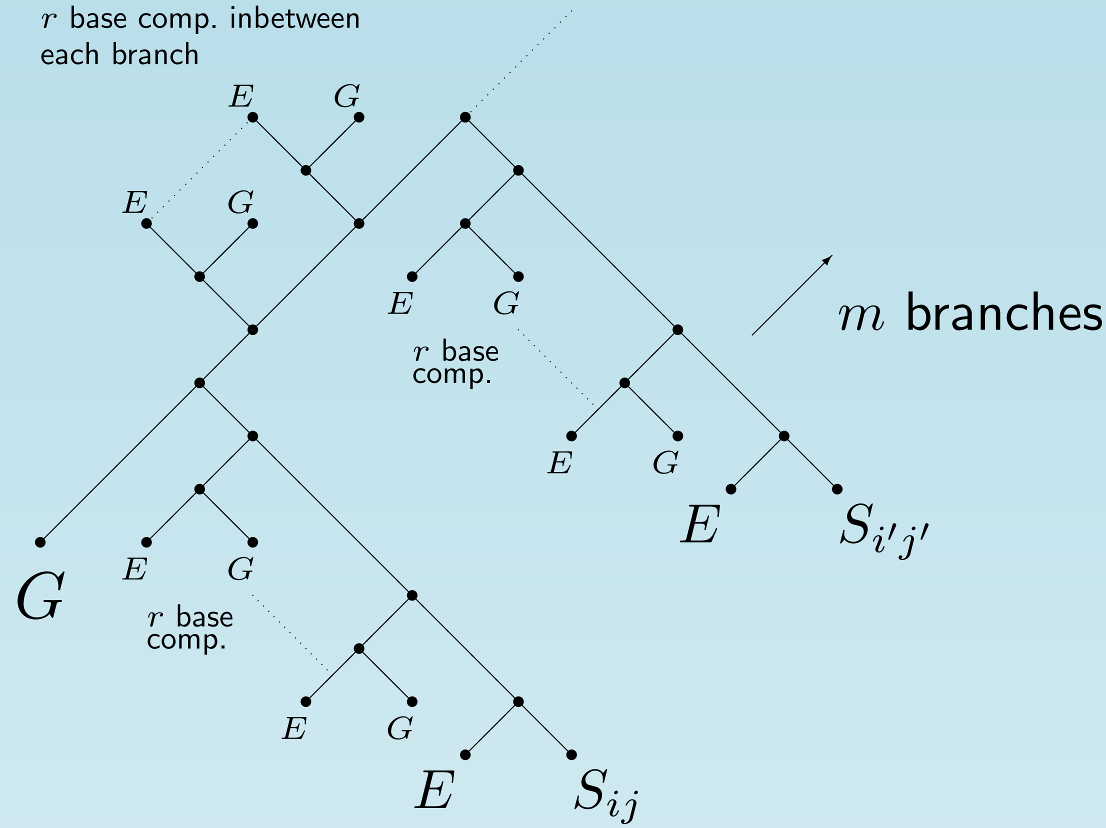


Symbol distance metric $\Longrightarrow$ Pairwise alignment distance metric

Tree Alignment is a special case of **Steiner Tree** in a metric space.

Construction Idea

Same idea as for STAR ALIGNMENT.



Overview and Open problems

Problem	Here	Approx
SP-score	all metrics	2-approx [GPBL]
Star Alignment	all metrics	2-approx
Tree Alignment (given phylogeny)	all metrics	PTAS [WJGL]

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SP-score	all metrics	2-approx [GPBL]
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Consensus Patterns	NP-hard	PTAS [LMW]
Substring Parsimony	NP-hard	PTAS [$\approx$ WJGL]

Acknowledgments

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Prof. Jens Lagergren

Prof. Benny for hosting me

Thanks!