A Simple Protocol for the Inference of RNA Global Pairwise Alignments

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Content

needle

Sequence Alignment

Needleman-Wunsch

LocARNA

Tree-based sequence

alignment

gardenia

RNA StrAT

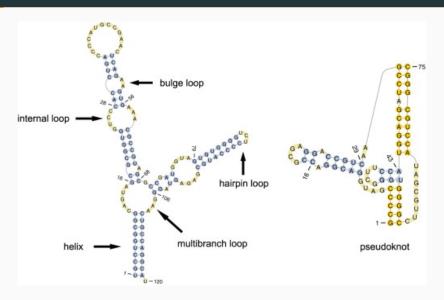
RNAdistance

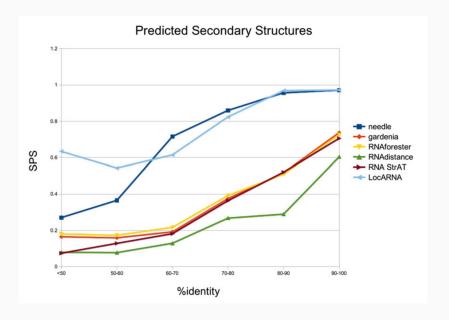
RNAforester

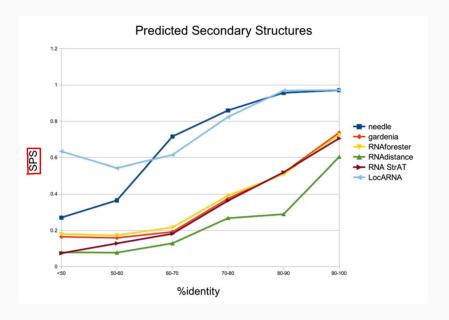
Comparison

Sources

RNA secondary structure







SPS - introduction

Sum of Pairs Score

SPS - introduction

Sum of Pairs Score

Used to measure the alignment of two RNA sequences

SPS - introduction

Sum of Pairs Score

Used to measure the similiarity of two RNA sequences

A: AAGGCTT

B: AAGGC

C: AAGGCAT

Similiarity:

A: AAGGCTT

B: AAGGC

C: AAGGCAT

Similiarity:

A: AAGGCTT

B: AAGGC

C: AAGGCAT

Similarity: 60% = 1 - (2 / 5)

A: AAGGCTT

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Similarity: 60% = 1 - (2 / 5)

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B: AAGGC

C: AAGGCAT

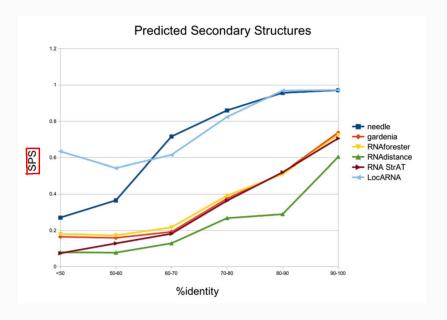
Similiarity:

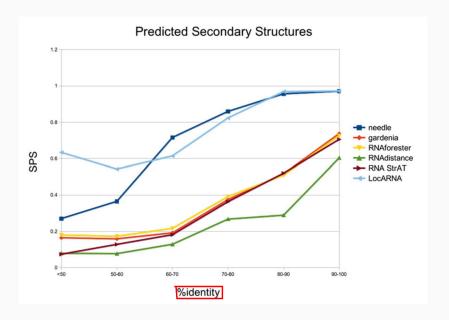
A: AAGGCTT

B: AAGGC

C: AAGGCAT

Similarity: 86% = 1 - (1 / 7)





A: AAGGCTT

B: AAGGC

C: AAGGCAT

Identity:

A: AAGGCTT

B: AAGGC

C: AAGGCAT

Identity:

A: AAGGCTT

B: AAGGC

C: AAGGCAT

Identity: 100%

A: AAGGCTT

B: AAGGC

C: AAGGCAT

Identity:

A: AAGGCTT

B: AAGGC

C: AAGGCAT

Identity: 100%

A: AAGGCTT

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C: AAGGCAT

Identity:

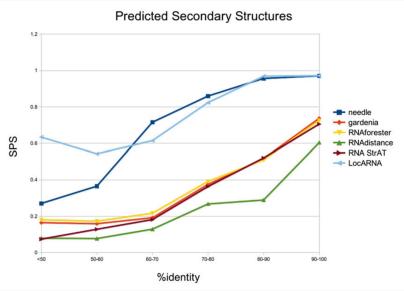
A: AAGGCTT

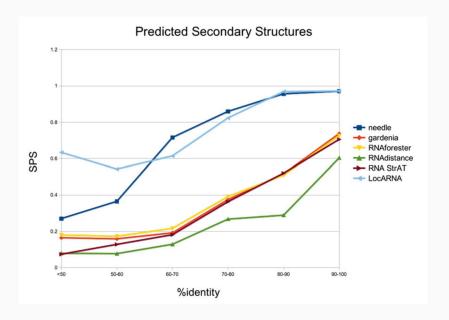
B: AAGGC

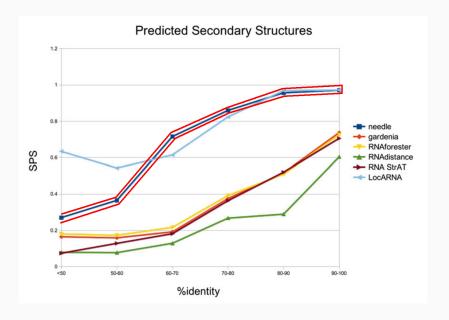
C: AAGGCAT

Identity: 85% = 6 / 7

Explain: predicted (RNAfold), test setup







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needle - Introduction

• Sequence based Algorithm

needle - Introduction

Sequence based Algorithm

• part of the EMBOSS package

needle - Introduction

• Sequence based Algorithm

part of the EMBOSS package

 Implementation of the Needleman-Wunsch algorithm

Needleman-Wunsch Algorithm

Sometimes also called:

Needleman-Wunsch Algorithm

Sometimes also called:

Optimal matching algorithm

Needleman-Wunsch Algorithm

Sometimes also called:

• Optimal matching algorithm

Global alignment technique

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• local sequence alignment

Sequence Alignment

• local sequence alignment

• global sequence alignment

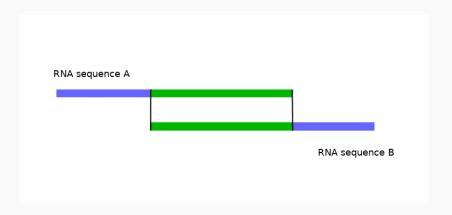
Sequence Alignment

local sequence alignment

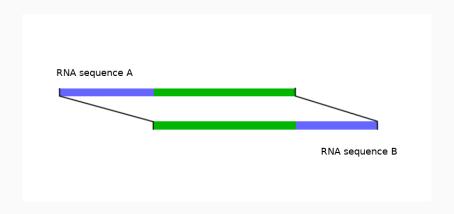
• global sequence alignment

glocal sequence alignment

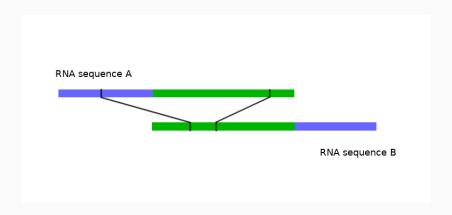
Sequence Alignment - local



Sequence Alignment - global



Sequence Alignment - glocal



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Needleman-Wunsch Algorithm - introduction

We need a scoring system.

Needleman-Wunsch Algorithm - introduction

We need a scoring system.

Example:

Needleman-Wunsch Algorithm - introduction

We need a scoring system.

Example:

- Match: 1
- Mismatch: -1
- Indel: -1

Needleman-Wunsch Algorithm

Two sequences to compare:

Needleman-Wunsch Algorithm

Two sequences to compare:

GCATGCU GATTACA

	G	С	Α	Т	G	С	U
G							
Α							
Т							
Т							
Α							
С							
Α							

		G	С	Α	Т	G	С	U
	0							
G								
Α								
Т								
Т								
Α								
С								
Α								

		G	С	Α	Т	G	С	U
	0	-1	-2	-3	-4	-5	-6	-7
G	-1							
Α	-2							
T	-3							
T	-4							
Α	-5							
С	-6							
A	-7							

		G	С	Α	Т	G	С	U
	0	-1	-2	-3	-4	-5	-6	-7
G	-1	Χ						
Α	-2							
T	-3							
T	-4							
Α	-5							
С	-6							
Α	-7							

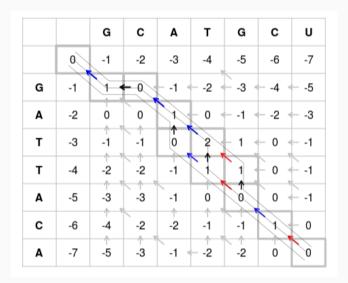
		G	С	Α	Т	G	С	U
	0	-1	-2	-3	-4	-5	-6	-7
G	-1	1						
Α	-2							
T	-3							
T	-4							
Α	-5							
С	-6							
Α	-7							

		G	С	Α	Т	G	С	U
	0	-1	-2	-3	-4	-5	-6	-7
G	-1	1	Χ					
Α	-2	Υ						
T	-3							
T	-4							
Α	-5							
С	-6							
Α	-7							

		G	С	Α	Т	G	С	U
	0	-1	-2	-3	-4	-5	-6	-7
G	-1	1	0					
Α	-2	0						
Т	-3							
Т	-4							
Α	-5							
С	-6							
Α	-7							

		G	С	Α	Т	G	С	U
	0	-1	-2	-3	-4	-5	-6	-7
G	-1	1	0	-1	-2	-3	-4	-5
Α	-2	0	0	1	0	-1	-2	-3
T	-3	-1	-1	0	2	1	0	-1
T	-4	-2	-2	-1	1	1	0	-1
Α	-5	-3	-3	-1	0	0	0	-1
С	-6	-4	-2	-2	-1	-1	1	0
Α	-7	-5	-3	-1	-2	-2	0	0

Needleman-Wunsch Algorithm - Best Matches



Needleman-Wunsch Algorithm - Results

Sequences	Best alignments					
GCATGCU	GCATG-CU	GCA-TGCU	GCAT-GCU			
GATTACA	G-ATTACA	G-ATTACA	G-ATTACA			

needle

Sequence Alignment

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Two steps:

Two steps:

 create base pair probability matrix using RNAfold

Two steps:

- create base pair probability matrix using RNAfold
- using these as guide for optimal alignment

Two steps:

- create base pair probability matrix using RNAfold
- using these as guide for optimal alignment

(folding and aligning)

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Sequence Alignment

Needleman-Wunsch

Locarna

Tree-based sequence alignment

gardenia

RNA StrAT

RNAdistance

RNAforester

Comparison

needle

Sequence Alignment

Needleman-Wunsch

Locarna

Tree-based sequence alignment

gardenia

RNA StrAT

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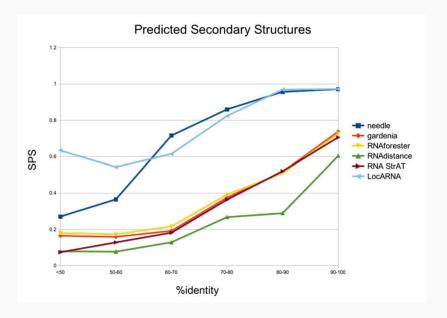
RNAforester

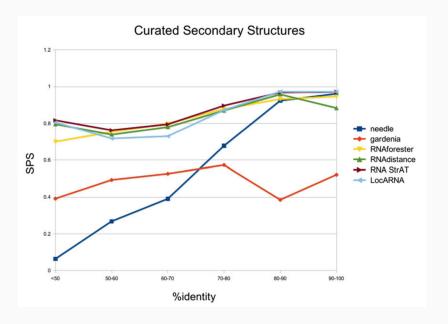
Comparison

Run time Comparison

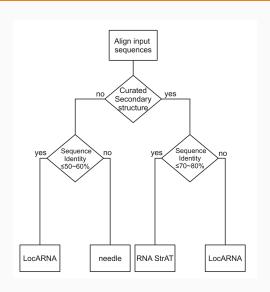
Mean running time (in seconds) per sequence

	bralibase	RNAspa	RNAstrand
needle	0.01	0.01	0.01
gardenia	0.01	0.01	0.02
RNA StrAT	0.02	0.32	0.46
LocARNA	0.02	0.08	0.02
RNAdistance	0.01	0.01	0.01
RNAforester	0.03	0.73	0.81





Proposed Workflow



needle

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Needleman-Wunsch

Locarna

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alignment

gardenia

RNA StrAT

RNAdistance

RNAforester

Comparison

Sources i

The slides can be found at:



https://github.com/fkarg/things-to-talk-about/tree/master/proseminar

Sources ii



https://upload.wikimedia.org/wikipedia/commons/3/3f/Needleman-Wunsch_pairwise_sequence_alignment.png

Secondary structures Image

https://www.sciencedirect.com/science/article/pii/B9780124200371000014