

Feng-Doolittle Unit Tests

Hint: Many test values are taken from project Algorithms for Bioninformatics of Alexander Mattheis or the lectures.

Test 1 (Hint: Notation from original paper! Formula was wrong! Mismatches were not considered!)

Input

Sequence a: ACGT
Sequence b: AT
Sequence c: GCC

Gap opening: 0 (can use Needleman-Wunsch instead of Gotoh)
Enlargement: -2
Match: 1 (and 0 for placeholder #)
Mismatch: -1

Output (Pairwise Alignment)

	Alignment- Length	Gaps	Gap- starts	Score
(a,b)	4	2	1	-2
(a,c)	4	1	1	-3
(b,c)	3	1	1	-4

Seq1 ACGT
 * *
Seq2 A__T

Seq1 ACGT
 |*|
Seq2 GC_C

Seq1 _AT
 ||
Seq2 GCC

Hint: More alignments exists, but only one is computed!

Output (Distances)

$$S_{a,b}^{rand} = \frac{1}{4} \left(\begin{array}{l} s(A_a, A_b) \cdot N_A(a) \cdot N_A(b) + s(A_a, T_a) \cdot N_A(a) \cdot N_T(b) \\ + s(C_a, A_b) \cdot N_C(a) \cdot N_A(b) + s(C_a, T_a) \cdot N_C(a) \cdot N_T(b) \\ + s(G_a, A_b) \cdot N_G(a) \cdot N_A(b) + s(G_a, T_b) \cdot N_G(a) \cdot N_T(b) \\ + s(T_a, A_b) \cdot N_T(a) \cdot N_A(b) + s(T_a, T_b) \cdot N_T(a) \cdot N_T(b) \end{array} \right)$$

+ 2 · enlarge

$$= \frac{1}{4} \left(\begin{array}{c} 1 + (-1) + (-1) + (-1) \\ + \\ (-1) + (-1) + (-1) + 1 \end{array} \right) + 2 \cdot (-2) = \frac{-4}{4} - 4 = -5$$

$$S_{a,b}^{max} = \frac{4 + 2}{2} = 3$$

$$S_{a,b}^{eff} = \frac{S(a,b) - S_{a,b}^{rand}}{S_{a,b}^{max} - S_{a,b}^{rand}} = \frac{-2 - (-5)}{3 - (-5)} = \frac{3}{8}$$

$$D(a,b) = -\ln S_{a,b}^{eff} \approx 0.98 \approx 1$$

$$S_{a,c}^{rand} = \frac{1}{4} \left(\begin{array}{l} s(A_a, G_b) \cdot N_A(a) \cdot N_G(b) + s(A_a, C_b) \cdot N_A(a) \cdot N_C(b) \\ + s(C_a, G_b) \cdot N_C(a) \cdot N_G(b) + s(C_a, C_b) \cdot N_C(a) \cdot N_C(b) \\ + s(G_a, G_b) \cdot N_G(a) \cdot N_G(b) + s(G_a, C_b) \cdot N_G(a) \cdot N_C(b) \\ + s(T_a, G_b) \cdot N_T(a) \cdot N_G(b) + s(T_a, C_b) \cdot N_T(a) \cdot N_C(b) \end{array} \right) + 1 \cdot enlarge$$

$$= \frac{1}{4} \left(\begin{array}{c} -1 + (-2) + (-1) + 2 \\ + \\ 1 + (-2) + (-1) + (-2) \end{array} \right) + 1 \cdot (-2) = \frac{-6}{4} - 2 = -3.5$$

$$S_{a,c}^{max} = \frac{4 + 3}{2} = 3.5$$

$$S_{a,c}^{eff} = \frac{S(a,c) - S_{a,c}^{rand}}{S_{a,c}^{max} - S_{a,c}^{rand}} = \frac{-3 - (-3.5)}{3.5 - (-3.5)} = \frac{0.5}{7}$$

$$D(a,c) = -\ln(S_{a,c}^{eff}) \approx 2.639 \approx 3$$

$$S_{b,c}^{rand} = \frac{1}{3} \cdot \left(\begin{array}{l} s(A_a, G_b) \cdot N_A(a) \cdot N_G(b) + s(A_a, C_b) \cdot N_A(a) \cdot N_C(b) \\ + s(T_a, G_b) \cdot N_T(a) \cdot N_G(b) + s(T_a, C_b) \cdot N_T(a) \cdot N_C(b) \end{array} \right) + 1 \cdot enlarge$$

$$= \frac{1}{3} \cdot (-1 + (-2) + (-1) + (-2)) - 2 = \frac{-6}{3} - 2 = -4$$

$$S_{b,c}^{max} = \frac{2 + 3}{2} = 2.5$$

$$S_{b,c}^{eff} = \frac{S(b,c) - S_{b,c}^{rand}}{S_{b,c}^{max} - S_{b,c}^{rand}} = \frac{-4 - (-4)}{2.5 - (-4)} = \frac{0}{6.5} \leq 0 \rightarrow S_{a,c}^{eff} = \frac{0.001}{6.5} = \frac{1}{6500}$$

$$D(b,c) = -\ln(S_{b,c}^{eff}) \approx 8.78 \approx 9$$

Output (Phylogenetic Tree)

1.

$$d_{min} = 1$$

	a	b	c
a	0	1	3
b		0	9
c			0

2.

$$\mathcal{C} = ((\mathcal{C} - \{a\}) - \{b\}) \cup \{d\}$$

	a	b	c	d
a	0	1	3	
b		0	9	
c			0	6
d				0

3.

$$\text{dist}(d, a) = \text{dist}(d, b) = \frac{1}{2} = 0.5$$

4.

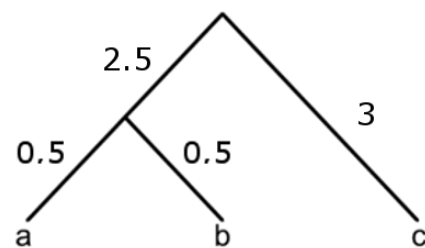
$$\text{dist}(c, d = \{a, b\}) = \frac{|a| \cdot \text{dist}(c, a) + |b| \cdot \text{dist}(c, b)}{|a| + |b|} = \frac{1 \cdot 3 + 1 \cdot 9}{1 + 1} = 6$$

1) $d_{min} = 6$

2) $\mathcal{C} = ((\mathcal{C} - \{c\}) - \{d\}) \cup \{e\}$

3) $\text{dist}(e, c) = \text{dist}(e, d) = \frac{d_{min}}{2} = 3$

	a	b	c	d	e
a	0	1	3		
b		0	9		
c			0	6	
d				0	
e					0



Hint: Tree is rounded, because of easiefied calculation!

Output (Joinment)

1.

ACGT

A##T

2.

ACGT GCC

A##T and

Seq1 ACGT

 |*|

Seq2 GC_C

Score -3

Seq1 ACGT

 |*|

Seq2 GCC_

Score -3

Hint: The following matrices are mirrored!

		A	#	#	T
	0	-2	-2	-2	-4
G	-2	-1	-1	-1	-3
C	-4	-3	-1	-1	-2
C	-6	-5	-3	-1	-2

Seq1 A##T

 | |

Seq2 G_CC

Score -2

		A	#	#	T
	0	-2	-2	-2	-4
G	-2	-1	-1	-1	-3
C	-4	-3	-1	-1	-2
C	-6	-5	-3	-1	-2

Seq1 A##T

 | |

Seq2 GC_C

Score -2

but: third alignment chosen, because highest score

Output (Final)

ACGT

A__T

G_CC

SoP-Score -11

Test 2 (Hint: Simulation with Gotoh)

Input

Sequence a: GCC

Sequence b: A##T

Gap opening: -1

Enlargement: -2

Match: 1 (and 0 for placeholder #)

Mismatch: -1

		A	#	#	T
		$-\infty$	$-\infty$	$-\infty$	$-\infty$
G	-	-6	-6	-6	-8
C	-	-4	-4	-4	-6
C	-	-6	-4	-4	-5

		A	#	#	T
	0	-3	-3	-3	-5
G	-3	-1	-1	-1	-3
C	-5	-4	-1	-1	-2
C	-7	-6	-4	-1	-2

		A	#	#	T
	0	-	-	-	-
G	$-\infty$	-5	-1	-1	-3
C	$-\infty$	-8	-4	-1	-3
C	$-\infty$	-10	-6	-4	-4

Seq1 GC_C

Seq2 A##T

Score -2

Seq1 G_CC

Seq2 A##T

(traceback not shown)

Score -2

(the neutral symbol # have only an effect on the two lower tables)