Feng-Doolittle Unit Tests

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

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

$$+ 2\cdot enlarge$$

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

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

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

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

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

$$=\frac{1}{4}\begin{pmatrix}-1+(-2)+(-1)+2\\ +\\ 1+(-2)+(-1)+(-2)\end{pmatrix}+1\cdot(-2)=\frac{-6}{4}-2=-3.5$$

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

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

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

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

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

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

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

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

Output (Phylogenetic Tree)

1.

$d_{min} = 1$

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

2.

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

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

3.

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

4.

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

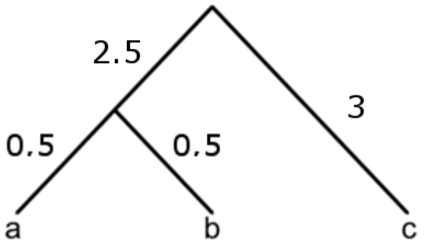
----

1) $d_{min} = 6$

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

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

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



Output (Joinment)

```
1.
ACGT
A##T

2.
ACGT        GCC
A##T   and

Seq1   ACGT          Seq1   ACGT
       |*  |                |*|
Seq2   GC_C          Seq2   GCC_
Score  -3            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
		-∞	-∞	-∞	-∞
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	-∞	-5	-1	-1	-3
C	-∞	-8	-4	-1	-3
C	-∞	-10	-6	-4	-4

```
Seq1  GC_C
      || |
Seq2  A##T
Score -2

Seq1  G_CC
      | ||  (traceback not shown)
Seq2  A##T
Score -2

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