

## Iterative Refinement Unit Tests

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

### Test 1 (used Feng-Doolittle implementation and Sum-of-Pairs implementation)

#### Input

Sequence a: ACGT  
Sequence b: AT  
Sequence c: GCT  
Sequence d: GC

Gap opening: -1  
Enlargement: -3  
Match: 1 (and 0 for placeholder #)  
Mismatch: 0

#### Output (Computation: Global Primary Library)

##### Feng-Doolittle Output

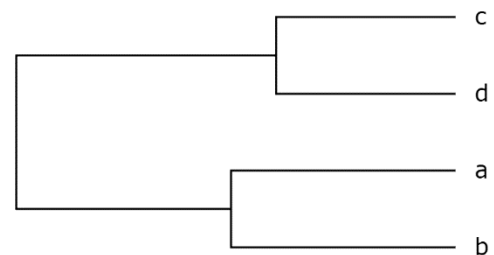
Alignment:

ACGT  
A\_\_T  
G\_CT  
G\_C\_

Distance-Table:

<b>D</b>	a	b	c	d
a	0	1.8	1.7	2.9
b	1.8	0	2.2	7.6
c	1.7	2.2	0	1.5
d	2.9	7.6	1.5	0

Tree:



#### Round-Robin – Minimum Distance Pair Output

Post-Order-Traversal: badc (left-right-root, where as in code reversed)

removed

sequence (Hint: is cleaned from gaps)

b:  $\operatorname{argmin}_x (D_{b,x}) = a$  with  $D_{b,a} = 1.8$

b~a: AT~ACGT

A\_\_T  
\*\_\_\*

ACGT

Nothing changes!

a:  $\operatorname{argmin}_x (D_{a,x}) = c$  with  $D_{a,c} = 1.7$

a~c: ACGT~GCT

ACGT  
|\*\_\*  
GC\_T

remaining

alignment

ACGT  
G\_CT  
G\_C\_

A\_\_T  
GCT

GC\_

(gap-only columns removed)

after realignment:

ACGT

A\_\_T

GC\_T

GC\_\_

Score: -26

Hint: This alignment is kept.

d:  $\operatorname{argmin}_x(D_{d,x}) = c$  with  $D_{d,c} = 1.5$

d~c: GC~GC#T

GC\_\_

\*\*

GC#T

ACGT

A\_\_T

GC\_T

Nothing changes!

Feng-Doolittle Alignment:

ACGT

A\_\_T

G\_CT

G\_C\_

Refined Realignment:

ACGT

A\_\_T

GC\_T

GC\_\_

**Round-Robin – Pairwise Best Pairs Output**

(analogous - but it is searched for the best and not the nearest alignment)

**Round-Robin – One-Vs-All Output**

(analogous - but it is searched for the best and not the nearest alignment)

The other used procedures are already have been already tested during T-Coffee and Feng-Doolittle.