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 #)

Distance-Table:

Mismatch: 0

Output (Computation: Global Primary Library)

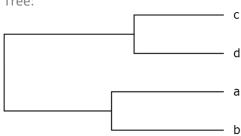
Feng-Doolittle Output

Alignment: ACGT

A__T G_CT G_C_

D	а	b	С	d
a	0	1.8	1.7	2.9
b	1.8	0	2.2	7.6

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

b~a: AT~ACGT

A__T

ACGT

Nothing changes!

a: $\underset{\chi}{\operatorname{argmin}}(D_{a,\chi}) = c \text{ with } D_{a,c} = 1.7$

 $\frac{\partial}{\partial x} \left(-u_{,x} \right) = 0$

a~c: ACGT~GCT

ACGT |* * GC_T

remaining

alignment

ACGT

G_CT G_C_

GCT

(gap-only columns removed)

after realignment:

ACGT $A__T$ GC_T GC__ Score: -26

This alignment is kept. Hint:

d:
$$\underset{x}{\operatorname{argmin}}(D_{d,x}) = c$$
 with $D_{d,c} = 1.5$ ACGT A__T GC_T

d~c: GC~GC#T

GC___

GC#T

Nothing changes!

Feng-Doolittle Alignment: Refined Realignment:

ACGT **ACGT** A__T G_CT A__T GC_T G_C_

Round-Robin - One-Vs-All

(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.