Bioinformatics I
WS 15/16
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1	2	3	$\sum$

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Assignment 4

(Abgabe am 9. November 2015)

Theoretical Assignment - *Optimal multiple alignment*

To calculate our MSA we use the recursion written down on page 50 in the script.

$$F(i_1,i_2,i_3) = max \begin{cases} F(i_1-1,i_2-1,i_3-1) + s_{SP}(a_{1i_1},a_{2i_2},a_{3i_3}) \\ \\ F(i_1-1,i_2-1,i_3) + s_{SP}(a_{1i_1},a_{2i_2},-) \\ F(i_1-1,i_2,i_3-1) + s_{SP}(a_{1i_1},-,a_{3i_3}) \\ F(i_1,i_2-1,i_3-1) + s_{SP}(-,a_{2i_2},a_{3i_3}) \\ \\ F(i_1-1,i_2,i_3) + s_{SP}(a_{1i_1},-,-) \\ F(i_1,i_2-1,i_3) + s_{SP}(-,a_{2i_2},-) \\ F(i_1,i_2,i_3-1) + s_{SP}(-,-,a_{3i_3}) \end{cases}$$

If we fill the DP matrix using this recursion, we get the following MSA:

$$\begin{pmatrix} C & T & T \\ - & T & C \\ C & C & T \end{pmatrix} \tag{1}$$

with score $\alpha_{SP}(A^*) = S(A,B) + S(A,C) + S(B,C) = -2 + 2 + (-6) = -6$.

Theoretical Assignment - *Progressive alignment*

The first step for the progressive alignment was to generate the pairwise global distance matrices. Afterwards the global optima were entered into a new table, which was used to generate the guide tree in the second step.(figure 3).

In step 2 the guide tree was created by the UPGMA methode in 3 substeps. After every step, which added a new cluster, the distance table was updated. The result from this step was the guide tree, which was used to apply the 'complete alignment' methode in the last step, the progressive alignment step.

Practical Assignment - *Comparing multiple alignment*

	0	C	T	T
0	0	-2	-4	-6
T	-2	-2	0	-2
C	-4	0	-2	-2

	0	C	T	T
0	0	-2	-4	-6
C	-2	2	0	-2
C	-4	0	0	-2
T	-6	-2	2	2

	0	C	T	T
0	0	-2	-4	-6
C	-2	2	0	-2
A	-4	0	0	-2
C	-6	-2	-2	-2
T	-8	-4	0	0

	0	T	C
0	0	-2	-4
C	-2	-2	0
C	-4	-4	0
T	-6	-2	-2

	0	T	C
0	0	-2	-4
C	-2	-2	0
A	-4	-4	-2
C	-6	-6	-2
T	-8	-8	-4

	0	C	C	T
0	0	-2	-4	-6
C	-2	2	0	-2
A	-4	0	0	-2
C	-6	-2	2	0
T	-8	-4	0	4

	A	B	C	D
A				
B	-2			
C	2	-2		
D	0	-4	4	

Figure 1: Global alignments lead to the basis table used to generate the guide tree

	A	B	C	D
A				
B	-2			
C	2	-2		
D	0	-4	4	

	A	B	CD
A			
B	-2		
CD	1	-3	

	ACD	B
ACD		
B	-5/3	

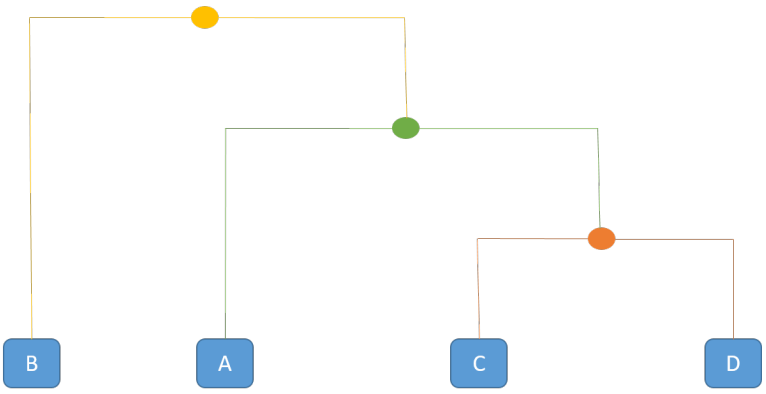
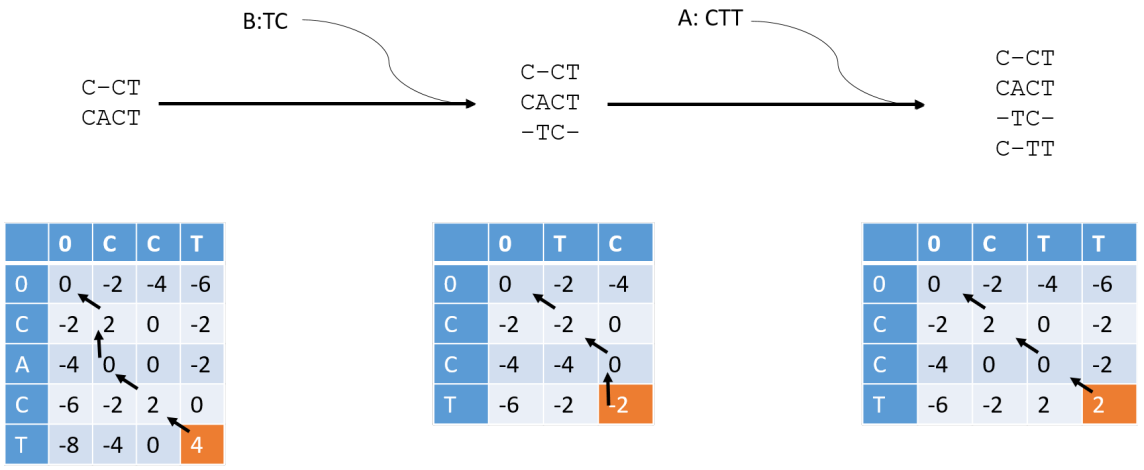


Figure 2: The guide tree is made from the final table from step 1



	0	C	C	T
0	0	-2	-4	-6
C	-2	2	0	-2
A	-4	0	0	-2
C	-6	-2	2	0
T	-8	-4	0	4

	0	T	C
0	0	-2	-4
C	-2	-2	0
C	-4	-4	0
T	-6	-2	-2

	0	C	T	T
0	0	-2	-4	-6
C	-2	2	0	-2
C	-4	0	0	-2
T	-6	-2	2	2

Figure 3: Complete alignment methode is used to get an MSA from the guidetree from step 2