# Evolutionary Thinking 2022 TA session week 1 – Alignment and Distance Matrix

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## Outline

1. Learning outcome of today (30 minutes)

Sequence Alignment

Distance Matrix

Examples: Manual align a pair sequence using dynamic progamming

3. Group Working on MEGA exercises (60 minutes)





Sequence Alignment

What are the materials that we need for doing a sequence alignment? (5 minutes discussion)





Sequence Alignment

What are the materials that we need for doing a sequence alignment? (5 minutes discussion)

- 1. Sequences (two or more)
- 2. Scoring system (From simple to complex)
- 3. Algorithms (Examples DP/Needleman and Wunsch)





Scoring system

Match + Mismatch -Gap -

Gap open – Gap continue -





DP/Needleman-Wunsch alignment – pairwise

C A T T A T C G C G T T - T C G

Global maximized alignment score max  $S_{1->x,1->y} = Max$  { max  $S_{1->x-1,1->y} + S_{x,y|x-1,y}$  max  $S_{1->x,1->y-1} + S_{x,y|x,y-1}$  max  $S_{1->x-1,1->y-1} + S_{x,y|x-1,y-1}$  }





Dynamic Programming alignment – pairwise

Match 5
Mismatch -3
Gap -4
Gap extension -1

		С	A	T	T	A	T	С	G
	0	0	0	0	0	0	0	0	0
C	0								
G	0								
T	0								
T	0								
T	0								
C	0								
G	0								





Match 5 Mismatch -3 Gap -4 Gap extension -1

Dynamic Programming alignment – pairwise

Group solving (15 minutes)

		С	A	T	T	A	T	С	G
	0	0	0	0	0	0	0	0	0
С	0								
G	0								
Т	0								
T	0								
T	0								
С	0								
G	0								





Match 5
Mismatch -3
Gap -4
Gap extension -1

Dynamic Programming alignment – pairwise

Group solving (15 minutes)

		С	A	T	T	A	T	С	G
	0	0	0	0	0	0	0	0	0
C	0	5	1 -	0	-1>	-2	-3	5	-1
G	0	1	2	-2	-3	-4	-5	1 1	10
T	0	0	-2	<b>*7</b>	3	2	1 -	0 *	6
T	0	-1	-3	<b>43</b>	12	8	7	6	5
T	0	-2 <sup>*</sup>	-4	2	8	9	13	9	8
C	0	5	1	1	7	5	9	18	14
G	0	1 *	2	0	6	4	8 •	14 🔻	23





Match 5
Mismatch -3
Gap -4
Gap extension -1

Dynamic Programming alignment – pairwise

Finding maximum

		C	A	T	T	A	T	С	G
	0	0	0	0	0	0	0	0	0
C	0	5	1 -	0	-1>	-2	-3	5	-1
G	0	1	2	-2	-3	-4	-5	1 '	10
T	0	0	-2	<b>*7</b>	3	2	1 -	0	6
T	0	-1	-3	<b>43</b>	12	8	7	6	5
T	0	-2 <sup>*</sup>	-4	2	8	9	13	9	8
C	0	5	1	1	7	5	9	18	14
G	0	1 *	2	0	6	4	8 •	14 ▼	23





Match 5
Mismatch -3
Gap -4
Gap extension -1

Dynamic Programming alignment – pairwise

#### Trace back

		С	A	T	T	A	T	C	G
	0	0	0	0	0	0	0	0	0
C	0	<b>5</b>	1	0	-1	-2	-3	5	-1
G	0	1 1	2	-2	-3	-4	-5	1 1	10
Т	0	0	-2	<b>47</b>	3	2	1 -	0 *	6
Т	0	-1	-3	<b>*3</b>	<b>112</b>	8	7	6	5
Т	0	-2 <sup>*</sup>	-4	<b>12</b>	18	9	13	9	8
C	0	5	1	1	7	5	9	18	14
G	0	1 *	2	0	6	4	8 •	14	23





Match 5
Mismatch -3
Gap -4
Gap extension -1

Dynamic Programming alignment – pairwise

Find alignment

		С	A	T	T	A	T	C	G
	0	<b>0</b>	0	0	0	0	0	0	0
С	0	5	1	0	<b>\</b> -1	-2	<b>~</b> 3	5	1
G	0	1	2	-2	<b>\_</b> -3	-4	<b>-</b> 5	1 🗼	10
T	0	0	-2	7	3	2	[1	0	6
T	0	-1	<b>~-3</b>	3	12	8	7	6	5
Т	0	-2	-4	2,	8	9	13	9	8
C	0	5	<b>1</b>	1,	7	5	9	18	74
G	0	1	2	0	6	4	8	14	23





Multiple Sequence Alignment – Extension of pair wise alignment (Graur P104-105)









