

INF281 Exercise 06

1. SP score

The SP (sum-of-pairs) score is used to evaluate multiple sequence alignments.

$$S(\mathcal{A}) = \sum_{i=1}^{m-1} \sum_{j=i+1}^m S(\bar{s}^i, \bar{s}^j)$$

Use the simple scoring scheme and the alignment \mathcal{A} to answer the following questions.

Alignment \mathcal{A} :

Seq1: A-G

Seq2: GCG

Seq3: G-T

Scoring scheme:

$R_{ab} = 1$ for $a = b$

$R_{ab} = 0$ for $a \neq b$

$g = 1$

N.B. The score of a column with two blanks in a pairwise alignment should be 0.

(a) Calculate the pairwise score $S(\bar{s}^1, \bar{s}^2)$.

(b) Calculate the pairwise score $S(\bar{s}^1, \bar{s}^3)$.

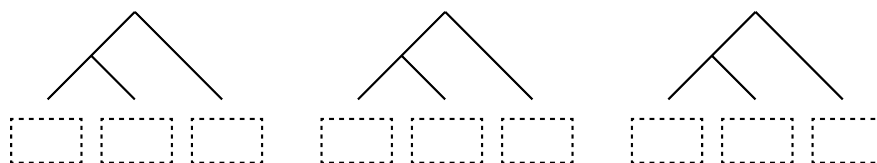
(c) Calculate the pairwise score $S(\bar{s}^2, \bar{s}^3)$.

(d) Calculate the SP score $S(\mathcal{A})$.

2. Tree topology

A rooted phylogenetic tree can have three topologically different trees when m is 3.

(a) Fill the labels A, B, or C to satisfy three topologically distinct trees.



3. UPGMA

UPGMA is an unweighted version of PGMA (pair-group method using arithmetic mean) for reconstructing a phylogenetic tree. Pairwise sequence alignments are used to calculate the distances among four sequences A, B, C, and D.

	A	B	C	D
A	0	2	7	7
B		0	5	9
C			0	8
D				0

Below are two examples of the distance calculation that can be used for UPGMA.

$$d_{(\alpha\beta),\gamma} = \frac{d_{\alpha,\gamma} + d_{\beta,\gamma}}{2}, \quad d_{(\alpha\beta\gamma),\delta} = \frac{d_{\alpha,\delta} + d_{\beta,\gamma} + d_{\delta,\gamma}}{3}$$

- (a) Identify the first internal node and update the distance matrix accordingly.

- (b) Identify the second internal node and update the distance matrix accordingly.

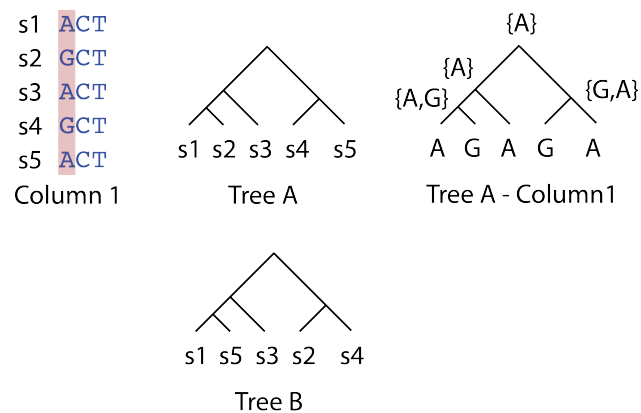
- (c) Reconstruct a rooted tree from the calculated distances.

- (d) Fill the distances of the reconstructed tree.

	A	B	C	D
A	0			
B		0		
C			0	
D				0

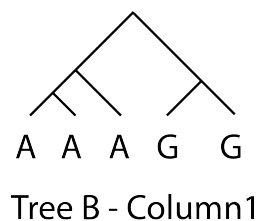
4. Maximum parsimony

The maximum parsimony uses column-wise operations of union and intersection. The number of union operations is counted to find the tree that minimizes the evolutionary changes.



Use the first column of the MSA and also Tree A and B to answer the following questions.

- How many union operations are necessary to estimate the labels of the root and the internal nodes of Tree A?
- Estimate the labels of the root and the internal nodes of Tree B.



- How many union operations are necessary to estimate the root and the internal nodes of Tree B?
- Which tree, Tree A or B, indicates less evolutionary changes when only the first column is considered?