

$$u_i^k = \sum_e f_{i,e}^k \quad C_{i,i}^k = \frac{1}{2} \left((u_i^k)^2 - \sum_e (f_{i,e})^2 \right) \quad C_{i,j,k}^k = u_i^k u_j^k - \sum_e f_{i,e}^k f_{j,e}^k \quad (17)$$

$$q_i = q_{i,i} + \frac{1}{2} \sum_{j \neq i} q_{i,j}$$

$$B_{i,j} = \begin{cases} 2 \log_2 (q_{i,i}/q_i^2) & i=j \\ 2 \log_2 (q_{i,j}/(2q_i q_j)) & i \neq j \end{cases}$$

Clusters

Blosum 100 \rightarrow 6 clusters

Blosum 7S \rightarrow 4 clusters $C_1 = \{1, 2, 3\}$ $C_2 = \{4\}$ $C_3 = \{5\}$ $C_4 = \{6\}$

K	A	C	G	T
1	4	0	2	0
2	2	0	0	4
3	0	0	4	2
4	0	0	5	1
5	5	0	0	1
6	4	1	0	1
7	1	0	0	5
8	0	6	0	0
9	0	5	0	1
10	3	1	0	2

$$\begin{aligned} & \cdot AA = 26 \\ & \cdot CC = 25 \\ & \cdot GG = 17 \\ & \Rightarrow \cdot TT = 18 \\ & \cdot CA/AC = 7 \\ & \cdot GA/AG = 8 \\ & \cdot TA/AT = 28 \\ & \cdot GC/CG = 0 \\ & \cdot TC/CT = 8 \\ & \cdot TG/GT = 13 \end{aligned}$$

$$\begin{aligned} L &= 10 \\ N &= 6 \\ E &= \frac{LN(N-1)}{2} = 150 \end{aligned}$$

$$q_{AA} = 26/150 = 0.1733$$

$$q_{AT} = 28/150 = 0.1867$$

$$q_{CG} = 0$$

$$q_{CC} = 0.167 [25/150]$$

$$q_{GG} = 0.114$$

$$q_{TT} = 0.12$$

$$q_{CA} = 0.044$$

$$q_{GA} = 0.053$$

$$q_{TA} = 0.187$$

$$q_{TC} = 0.053$$

$$q_{TG} = 0.087$$

Always taking the combination of combinations by 150

$$\begin{aligned} q_A &= 0.1733 + \frac{1}{2} (0.0467 + 0.0533 + 0.1867) = 0.3167 \\ q_C &= 0.2167 \quad q_G = 0.1833 \quad q_T = 0.2833 \end{aligned}$$

$$\begin{aligned} B_{AA} &= 2 \log_2 (0.1733/0.3167^2) = 1.57 \text{ p.u.} \\ B_{AC} &= 2 \log_2 (0.0467/(2 \cdot 0.3167 \cdot 0.2167)) \approx -3 \end{aligned}$$

\downarrow Blosum 100 (rounded)

A	C	G	T
A	-2	-3	-2
C	-3	4	-10
G	-2	-10	4
T	0	-2	-1

BLOSUM 75

$$C_1 = \{1, 2, 3\} \rightarrow \text{only mix cd} \quad K6 \quad A = 2/3 \quad T = 1/3 \\ K10 \quad A = 2/3 \quad C = 1/3$$

$$AA = 8 \quad CC = 9 \quad GG = 5 \quad TT = 6$$

$$CA/AC = 3 \quad GA/AG = 4 \quad TA/AT = 14 \quad GC/CG = 0$$

$$TC/CT = 4 \quad TG/GT = 7$$

$$\text{so I have } L = 10 \quad N = 4 \text{ (cluster)} \rightarrow z = (0.4 \cdot 3)/2 = 6^\circ$$

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$$q_{AA} = 8/60 = 0.1333 \quad q_{AT} = 14/60 = 0.2333 \quad q_{CG} = 0$$

$$q_A = 0.3083 \quad q_C = 0.2083 \quad q_G = 0.175 \quad q_T = 0.3083$$

↗ BLOSUM 75 (rounded)

	A	C	G	T	
A	1	-3	-1	1	
C	-3	4	-10	-2	
G	-1	-10	3	0	
T	1	-2	0	0	