

This document sketches out the objective function and gradient used to find the maximum likelihood reversible count matrix.

Let  $C_{ij}$  be the matrix of observed counts.  $C$  must be strongly connected for this approach to work! Below,  $f$  is the log likelihood of the observed counts.

$$f = \sum_{ij} C_{ij} \log T_{ij} \quad (1)$$

$$\text{Let } T_{ij} = \frac{X_{ij}}{\sum_j X_{ij}}, X_{ij} = \frac{1}{Z} \exp(u_{ij}), q_i = \sum_j \exp(u_{ij})$$

$$f = \sum_{ij} C_{ij} u_{ij} - \sum_{ij} C_{ij} \log q_i \quad (2)$$

$$\text{Let } N_i = \sum_j C_{ij}$$

$$f = \sum_{ij} C_{ij} u_{ij} - \sum_i N_i \log q_i \quad (3)$$

Let  $u_{ij} = u_{ji}$  for  $i > j$ , eliminating terms with  $i > j$ .

$$\text{Let } S_{ij} = C_{ij} + C_{ji}$$

$$f = \sum_{i \leq j} S_{ij} u_{ij} - \frac{1}{2} \sum_i S_{ii} u_{ii} - \sum_i N_i \log q_i \quad (4)$$

$$\frac{df}{du_{ab}} = S_{ab} - \frac{1}{2} S_{ab} \delta_{ab} - \sum_i \frac{N_i}{q_i} \frac{dq_i}{du_{ab}}$$

$$\frac{dq_i}{du_{ab}} = \exp(u_{ab}) [\delta_{ai} + \delta_{bi} - \delta_{ab} \delta_{ia}]$$

$$\text{Let } v_i = \frac{N_i}{q_i}$$

$$\sum_i V_i \frac{dq_i}{du_{ab}} = \exp(u_{ab}) (v_a + v_b - v_a \delta_{ab})$$

Thus,

$$\frac{df}{du_{ab}} = S_{ab} - \frac{1}{2} S_{ab} \delta_{ab} - (v_a + v_b - v_a \delta_{ab}) \quad (5)$$