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.

$$f = \sum_{ij} C_{ij} \log T_{ij}$$

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

$$f = \sum_{ij} C_{ij} u_{ij} - \sum_{ij} C_{ij} \log q_i$$

Let $N_i = \sum_j C_{ij}$

$$f = \sum_{ij} C_{ij} u_{ij} - \sum_{i} N_i \log q_i$$

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

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

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

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

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,

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