1 Intro

Here are the self-consistent equations:

$$f_i = -\log \sum_j \frac{\exp[-u_i(x_j)]}{\sum_k N_k \exp[f_k - u_k(x_j)]}$$

$$c_i = \sum_j \frac{q_i(x_j)}{\sum_k N_k c_k^{-1} q_k(x_j)}$$

2 Exp Space

Let

$$Q_{ij} = q_i(x_j)$$

and

$$R_{ij} = Q_{ij} N_i$$

Then

$$c_i = \sum_j \frac{Q_{ij}}{\sum_k R_{kj} c_k^{-1}}$$

3 Log Space

Let's work out an optimized form of the log-space calculation.

Let

$$\mu_{ij} = \log(N_i) - u_i(x_j)$$

Thus

$$f_i = -\log \sum_j \frac{\exp[-u_i(x_j)]}{\sum_k \exp[f_k + \mu_{kj}]}$$

$$f_i = -\log \sum_j \exp[-u_i(x_j) - \log \sum_k \exp[f_k + \mu_{kj}]]$$

Thus, we need to perform two logsumexp calculations:

$$s_j = -\log \sum_k \exp[f_k + \mu_{kj}]$$

$$f_i = -\log \sum_j \exp[-u_i(x_j) + s_j]$$

4 Minimization

Consider the objective function:

$$F = \sum_k^K N_k f_k - \sum_n^N \log \sum_k N_k \exp(f_k - u_k(x_n))$$

The partial derivatives are given by

$$\frac{\partial F}{\partial f_i} = N_i - \sum_n N_i \exp(f_i) \exp(-u_i(x_n)) \frac{1}{\sum_k N_k \exp(f_k - u_k(x_n))}$$

$$\frac{\partial F}{\partial f_i} = N_i - N_i \exp(f_i) \sum_n \exp(-u_i(x_n)) \frac{1}{\sum_k N_k \exp(f_k - u_k(x_n))}$$

Suppose we solve for the maximum of this equation:

$$\frac{\partial F}{\partial f_i} = 0$$

$$N_i = N_i \exp(f_i) \sum_n \exp(-u_i(x_n)) \frac{1}{\sum_k N_k \exp(f_k - u_k(x_n))}$$

$$\exp(-f_i) = \sum_n \exp(-u_i(x_n)) \frac{1}{\sum_k N_k \exp(f_k - u_k(x_n))}$$

$$f_i = -\log \sum_n \exp(-u_i(x_n)) \frac{1}{\sum_k N_k \exp(f_k - u_k(x_n))}$$

Thus, the maximization problem encodes the MBAR equations. Now, how does one best calculate the gradient?

$$\frac{\partial F}{\partial f_i} = N_i - \sum_n N_i \exp(f_i) \exp(-u_i(x_n)) \frac{1}{\sum_k N_k \exp(f_k - u_k(x_n))}$$

As we saw previously, we can decompose this into two *logsumexp* calculations– first the denominator, then the numerator. Again, this approach should be fairly robust as the logsumexp operation limits overflow error.