MBAR の実装

$$\hat{f}_i = -\ln \sum_{j=1}^{K} \sum_{n=1}^{N_j} \frac{\exp\left[-u_i(x_{jn})\right]}{\sum_{k=1}^{K} N_k \exp\left[\hat{f}_k - u_k(x_{jn})\right]}$$

$$= -\ln \sum_{j=1}^{K} \sum_{n=1}^{N_j} \frac{1}{\sum_{k=1}^{K} N_k \exp\left[\hat{f}_k - u_k(x_{jn}) - u_i(x_{jn})\right]}$$

$$= -\ln \sum_{j=1}^{K} \sum_{n=1}^{N_j} W_{jn}^{(i)}$$

$$= -\ln \sum_{i=1}^{K} \sum_{n=1}^{N_j} \exp\left[\ln W_{jn}^{(i)}\right]$$

$$= -\underset{i=1,K \quad n=1,N_j}{\text{logsumexp}} \ln W_{jn}^{(i)}$$

where

$$W_{jn}^{(i)} = \frac{1}{\sum_{k=1}^{K} N_k \exp\left[\hat{f}_k - u_k(x_{jn}) - u_i(x_{jn})\right]}$$

$$\ln W_{jn}^{(i)} = -\ln \left\{ \sum_{k=1}^{K} N_k \exp\left[\hat{f}_k - u_k(x_{jn}) - u_i(x_{jn})\right] \right\}$$

$$= -\ln \sum_{k=1}^{K} \exp\left[\ln N_k + \hat{f}_k - u_k(x_{jn}) - u_i(x_{jn})\right]$$

$$= -\underset{k=1,\ldots,K}{\text{logsumexp}} \left[\ln N_k + \hat{f}_k - u_k(x_{jn}) - u_i(x_{jn})\right]$$