

MBAR

1/2

$$F_1 = -\beta^{-1} \ln Z_1 = -\beta^{-1} \ln \int e^{-\beta U_1(x)} dx \approx -\beta^{-1} \ln \sum_{n=1}^N e^{-\beta U_1(x_n)}$$

$$F_2 = -\beta^{-1} \ln Z_2 = -\beta^{-1} \ln \int e^{-\beta U_2(x)} dx \approx -\beta^{-1} \ln \sum_{n=1}^N e^{-\beta U_2(x_n)}$$

$$F_3 = -\beta^{-1} \ln Z_3 = -\beta^{-1} \ln \int e^{-\beta U_3(x)} dx \approx -\beta^{-1} \ln \sum_{n=1}^N e^{-\beta U_3(x_n)}$$

例 1

F_1, F_2, F_3 を精度良く求める. $mbar()$ を使, 2つは
絶対値は求めず $F_1 = 0$ として相対値を求める

例 2

F_3 は target として $U_{\text{target}} = U_3$ のパラメータ θ_{target} を推定する.

$mbar-f()$ の引数は $F_0 = mbar-f(u_{kl}, [F_1, F_2], u_0)$

これは loss 関数は

$$Loss(\theta) = [F_3 - mbar-f(u_{kl}, [F_1, F_2], u_0)]^2$$

mean f() の中身

$$F_{\theta} = -\ln \sum_{j=1}^2 \sum_{n=1}^{N_j} \frac{\exp[-u_{\theta}(x_{j,n})]}{\sum_{k=1}^2 N_k \exp[\hat{F}_k - u_k(x_{j,n})]} = -\ln \sum \sum W \quad 2/2$$

$$\frac{\partial F_{\theta}}{\partial u_{\theta}(x_{j',n'})} = -\frac{\partial}{\partial u_{\theta}} \ln \sum \sum W = -\frac{1}{\sum \sum W} \times \frac{\partial}{\partial u_{\theta}(x_{j',n'})} \sum \sum W$$

$$= -\sum \sum W \times \frac{\partial}{\partial u_{\theta}(x_{j',n'})} \sum_{j=1}^2 \sum_{n=1}^{N_j} \frac{\exp[-u_{\theta}(x_{j,n})]}{\sum_{k=1}^2 N_k \exp[\hat{F}_k - u_k(x_{j,n})]}$$

$$= + \sum \sum W \times \frac{\exp[-u_{\theta}(x_{j',n'})]}{\sum_{k=1}^2 N_k \exp[\hat{F}_k - u_k(x_{j',n'})]}$$

$$= \exp(-F_{\theta}) \times w_{j',n'}$$