Exponetial Averaging (Reweightingの一種)

$$F = -\beta^{-1} \ln Z = -\beta^{-1} \ln \int e^{-\beta U(x)} dx$$

$$F_{target} = -\beta^{-1} \ln Z_{target} = -\beta^{-1} \ln \int e^{-\beta U_{target}(x)} dx$$

$$F_{target} - F = -\beta^{-1} \left[\ln Z_{target} - \ln Z \right] = -\beta^{-1} \ln \frac{Z_{target}}{Z}$$

$$= -\beta^{-1} \ln \frac{\int e^{-\beta U_{target}(x)} dx}{Z} = -\beta^{-1} \ln \frac{\int e^{-\beta U_{target}(x) + \beta U(x) - \beta U(x)} dx}{Z}$$

$$= -\beta^{-1} \ln \left\langle e^{-\beta(U_{target}(x) - U(x))} \right\rangle = -\beta^{-1} \ln \left\langle e^{-\beta \Delta U(x)} \right\rangle$$

やること 1 F_{target} と F を精度よく求める. $\Delta U(x) \equiv U_{target}(x) - U(x)$

$$F \approx -\beta^{-1} \ln \frac{1}{N} \sum_{n=1}^{N} e^{-\beta(x_n)} \qquad F_{target} \approx -\beta^{-1} \ln \frac{1}{N} \sum_{n=1}^{N} e^{-\beta U_{target}(x_n)}$$

やること 2 F_{target} と F の MSE から U_{target} のパラメータを推定

$$(F_{target} - F)^2 \approx \left(-\beta^{-1} \ln \frac{1}{N} \sum_{n=1}^{N} e^{-\beta \Delta U(x_n)} \right)^2$$