Reweighting methods for Monte Carlo data

Jonas Schaible

Institute of Theoretical Physics

Goethe University Frankfurt

JOHANN WOLFGANG GOETHE
UNIVERSITÄT
FRANKFURT AM MAIN

June 20, 2025

Monte Carlo simulations

Canonical partition function and ensemble average

$$Z = \sum_n e^{-\beta E_n}$$

$$\mathcal{O} = \frac{1}{Z} \sum_n O_n e^{-\beta E_n}$$

Coupling : β
Conjugate energy : E

Ising

$$E\{s_i\} = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^{N} s_i$$

$$Z(H,T) = \sum_{\{s_i\}} e^{-\beta E\{s_i\}}$$

QCD (N_f degenerate quarks)

$$Z = \int D[U] \, (det \, \mathsf{D}[U])^{N_f} \, e^{-S_g[U]}$$

$$S_G[U] = \beta \sum_{n \in \Lambda} \sum_{\mu < \nu} \left(1 - \frac{1}{N} Re\{tr \, U_{\mu\nu}(n)\} \right)$$

Monte Carlo simulations

- Sum over small subset
- Subset chosen from probability distribution p_n
- Importance sampling

$$\mathcal{O}_N(\beta) = \frac{\sum_{n=1}^{N} \mathcal{O}_n \, p_n^{-1} \, e^{-\beta E_n}}{\sum_{n=1}^{N} p_n^{-1} \, e^{-\beta E_n}}$$

$$p_n = \frac{1}{Z} e^{-\beta E_n}$$

$$\mathcal{O}_N(\beta) = \frac{1}{N} \sum_{n=1}^{N} \mathcal{O}_n$$

Reweighting

- Expand Monte Carlo results to different parameter values
- Ferrenberg and Swendsen: single & multiple histogram reweighting
- Single histogram reweighting: extrapolation from one simulated coupling value
- Multiple histogram reweighting: interpolation between several simulated coupling values

Single histogram reweighting

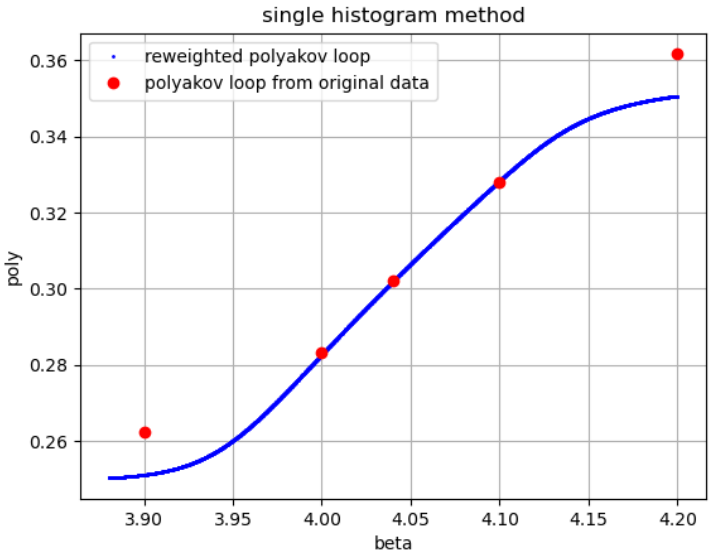
Monte Carlo estimator:

$$\mathcal{O}_N(\beta) = \frac{\sum_{n=1}^{N} \mathcal{O}_n \, p_n^{-1} \, e^{-\beta E_n}}{\sum_{n=1}^{N} p_n^{-1} \, e^{-\beta E_n}}$$

Boltzmann weight at β_0

$$p_n = \frac{1}{Z_0} e^{-\beta_0 E_n}$$

$$\mathcal{O}_N(\beta) = \frac{\sum_{n=1}^{N} \mathcal{O}_n \, e^{-(\beta-\beta_0) E_n}}{\sum_{n=1}^{N} e^{-(\beta-\beta_0) E_n}}$$



Multiple histogram reweighting

$$Z(\beta) = \sum_{i,n} \frac{1}{\sum_j N_j \, Z_j^{-1} \, e^{(\beta-\beta_j)E_{i,n}}}$$

$$\mathcal{O}_N(\beta) = \frac{1}{Z(\beta)} \sum_{i,n} \frac{\mathcal{O}_{i,n}}{\sum_j N_j \, Z_j^{-1} \, e^{(\beta-\beta_j)E_{i,n}}}$$

Large $n_j(E)$ leads to a good approximation of $\rho(E)$
→ large overlap of histogram

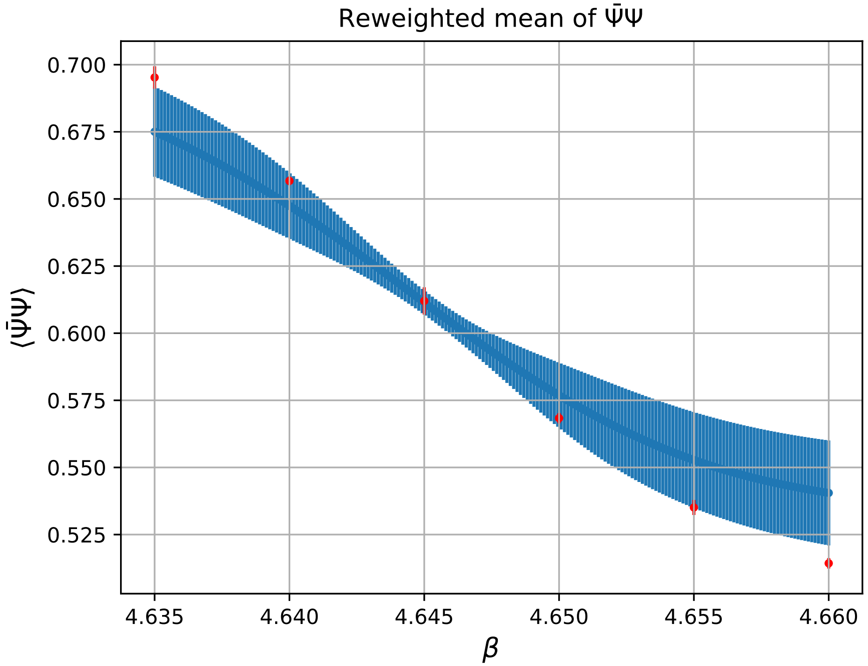
- Multiple histogram method with one β → single histogram method
- Error calculation: Bootstrap
- Multiple couplings:

$$Z(\beta) = \sum_{i,n} \frac{1}{\sum_j N_j \, Z_j^{-1} \, e^{\sum_\alpha (J_\alpha - J_{\alpha,j})E_{\alpha,i,n}}}$$

$$\mathcal{O}_N(\beta) = \frac{1}{Z(\beta)} \sum_{i,n} \frac{\mathcal{O}_{i,n}}{\sum_j N_j \, Z_j^{-1} \, e^{\sum_\alpha (J_\alpha - J_{\alpha,j})E_{\alpha,i,n}}}$$

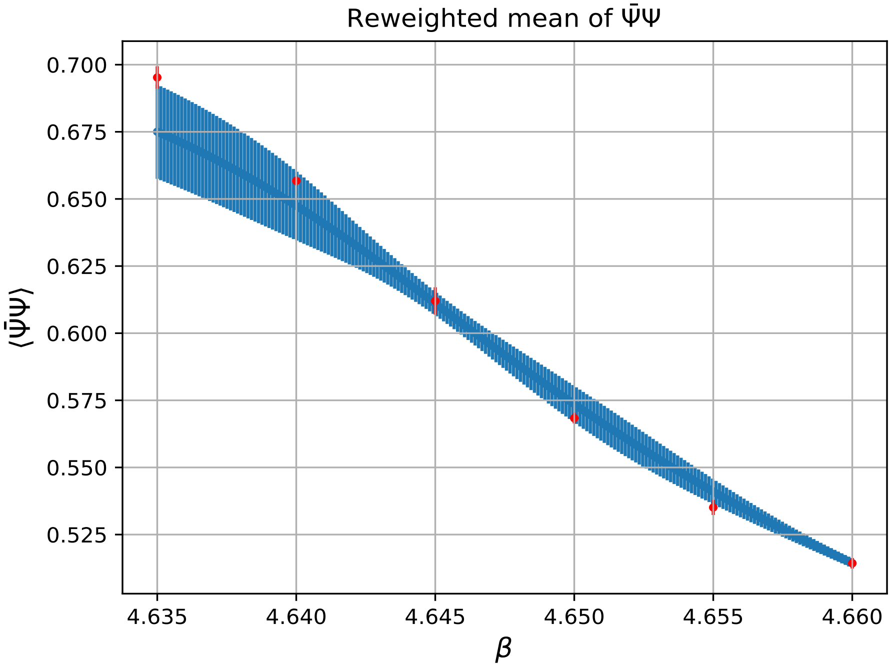
Single vs Multiple histogram reweighting

Single histogram



$\beta_{sim} = 4.645$

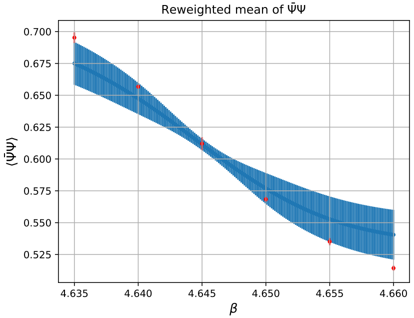
Multiple histogram



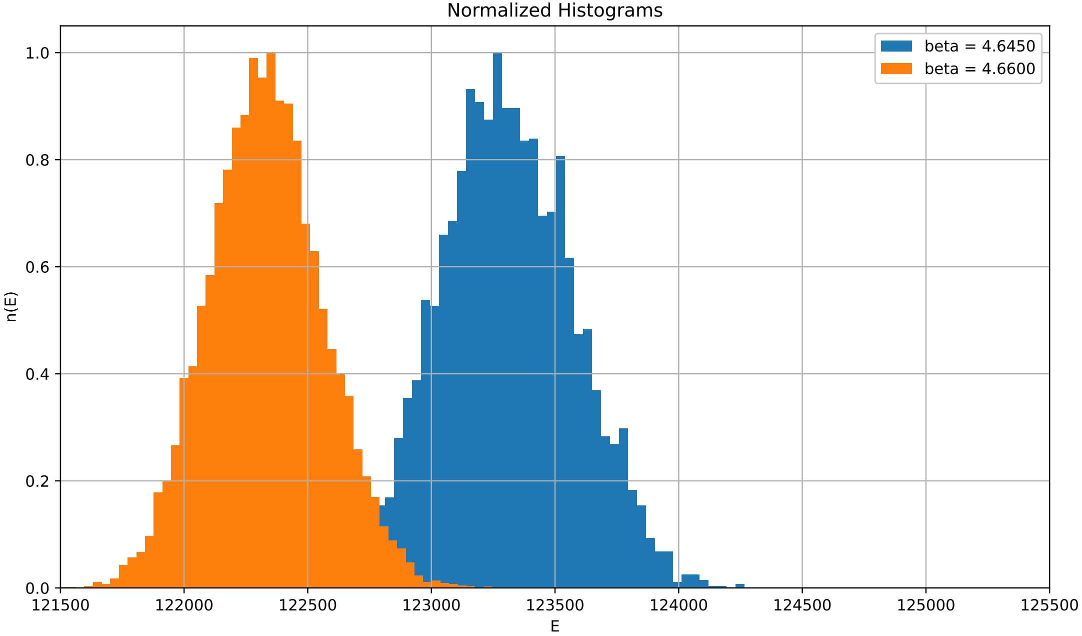
$\beta_{sim} = 4.645 , 4.660$

Single vs Multiple histogram reweighting

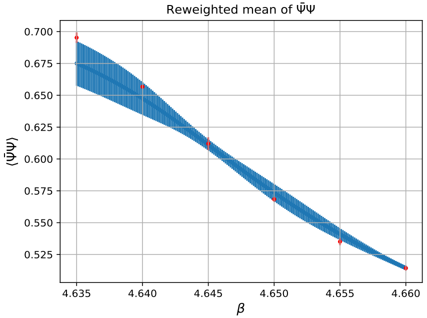
Single histogram



$\beta_{sim} = 4.645$

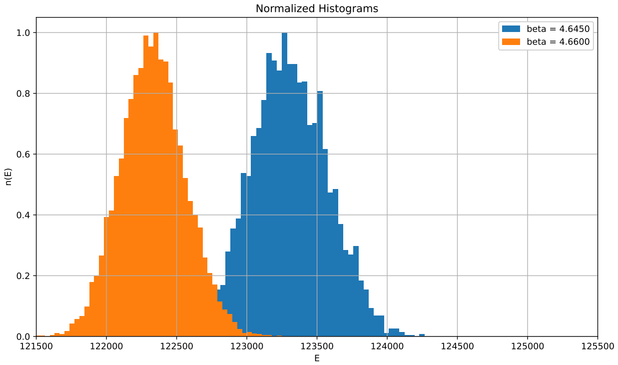


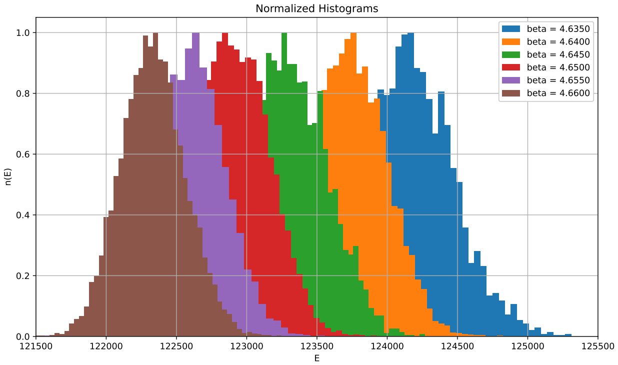
Multiple histogram

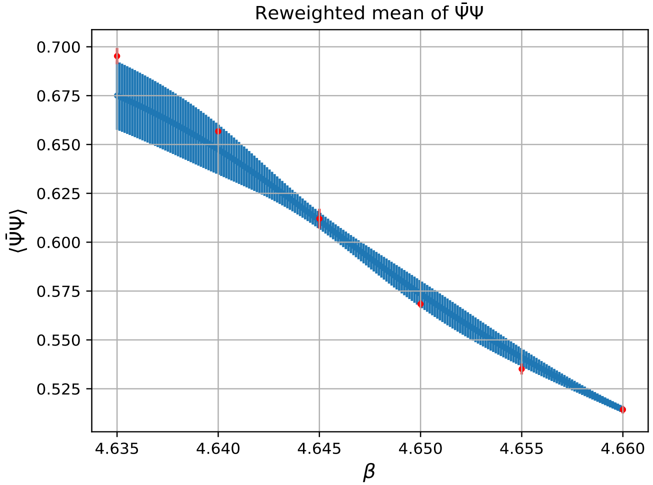


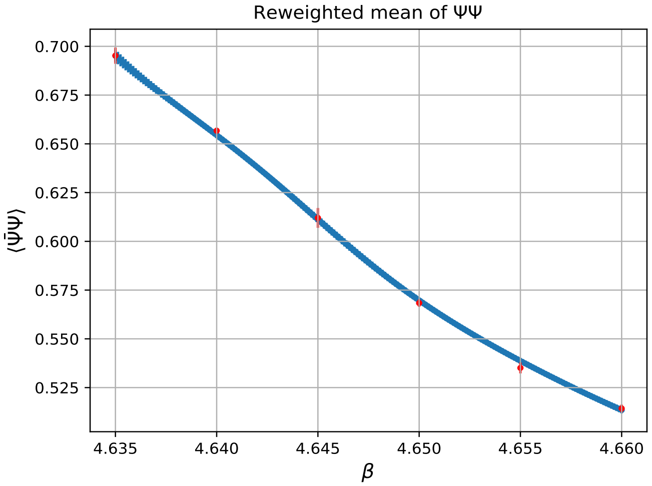
$\beta_{sim} = 4.645 , 4.660$

Multiple histogram reweighting



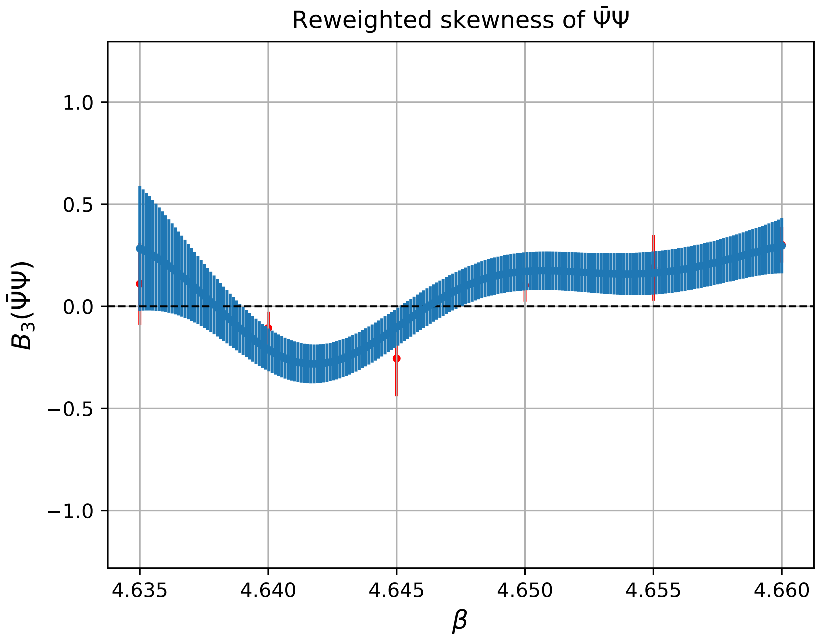


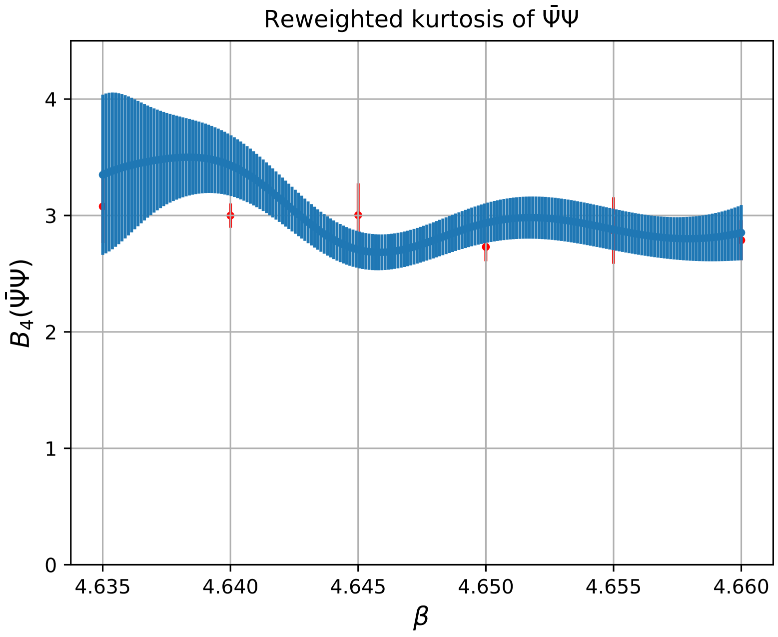




Multiple histogram reweighting

- Higher moments usefull for finding β_c





Logarithmic summation

- Avoid numerical overflow/underflow
- Exponent always ≤ 0 for a ≥ b
- Partition function and estimator

$$\ln(a+b) = \ln\left(e^{\ln(a)} + e^{\ln(b)}\right) = \ln(a) + \ln\left(1 + e^{\ln(b)-\ln(a)}\right)$$

$$\ln\left(\sum_i x_i\right) = \ln\left(x_{max} + \sum_{i \neq max} x_i\right) = \ln\left(e^{ln(x_{max})} + \sum_{i \neq max} e^{\ln(x_i)}\right)$$

$$= \ln(x_{max}) + \ln\left(1 + \sum_{i \neq max} e^{\ln(x_i) - \ln(x_{max})}\right)$$

$$\ln(Z_k) = \ln\left(\sum_l X_l(\beta_k)\right) = \ln\left(\sum_l e^{\ln(X_l(\beta_k))}\right)$$

$$\ln(X_l(\beta_k)) = -\ln\left(\sum_j e^{\ln(N_j) + (\beta_k - \beta_j)E_l - \ln Z_j}\right).$$

$$\mathcal{O}(\beta) = e^{\ln\left(\sum_l \mathcal{O}_l \cdot X_l(\beta)\right) - \ln(Z(\beta))}$$

Iteration of Z_k

$$Z_k = \sum_{i,n} \frac{1}{\sum_j N_j \, e^{(\beta_k - \beta_j)E_{i,n} - ln(Z_j)}}$$

$$Z_k = 1 \rightarrow ln(Z_k) = 0$$

- Partition function self-consistent
- Newton-Raphson method for better convergence behavior

Newton-Raphson method

- Multiple dimensions
- Taylor expansion around the root of $f_k(x)$

$$0 = f_k(\vec{x}^{(n)} + \vec{\delta}) = f_k(\vec{x}^{(n)}) + \left.\frac{\partial f_k(\vec{x})}{\partial x_m}\right|_{\vec{x}=\vec{x}^{(n)}} \delta_m + \mathcal{O}(\delta^2) \approx f_k(\vec{x}^{(n)}) + J_{km}\Delta x_m \qquad J_{km} = \frac{\partial f_k}{\partial x_m}$$

- System of linear equations

$$-f_k(x^{(n)}) = J_{km}\Delta x_m$$

- Update step

$$\vec{x}^{(n+1)} = \vec{x}^{(n)} + \Delta\vec{x}$$

- Jacobian has to be know analytically or cheap to evaluate

Newton-Raphson method

Find root of

$$f(ln(Z_k)) = ln\left(\sum_{i,n} \frac{1}{\sum_j N_j\, Z_j^{-1}\, e^{(\beta_k-\beta_j)E_{i,n}}}\right) - ln(Z_k) \qquad J_{km} = \frac{\partial f(ln(Z_k))}{\partial ln(Z_m)}$$

$$J_{km} = exp\left\{-ln(Z_m) + ln\left(\sum_{i,n} N_m\, e^{(\beta_k-\beta_m)E_{in}+2ln(X_{i,n}(\beta_k))}\right) - ln\left(\sum_{i,n} e^{ln(X_{i,n}(\beta_k))}\right)\right\} - \delta_{km}$$

$$-f(ln(Z_k)) = J_{km}\Delta ln(Z_m) \qquad ln(Z_k^{(n+1)}) = ln(Z_k^{(n)}) + \Delta ln(Z_k)$$

Newton-Raphson method

- Iterate until desired precision is reached

$$\Delta_n^2 = \sum_k \left(\frac{Z_k^{(n)} - Z_k^{(n-1)}}{Z_k^{(n)}} \right)^2 = \sum_k \left(1 - e^{-\Delta ln Z_k}\right)^2 \leq precision^2$$

- Damping factor can be introduced

$$\ln\left(Z_k^{(n+1)}\right) = \ln\left(Z_k^{(n)}\right) + \lambda \cdot \Delta \ln(Z_k)$$

- Partition function can be rescaled by a constant

$$Z_k = \sum_{i,n} \frac{1}{\sum_j N_j \, Z_j^{-1} \, e^{(\beta_k - \beta_j) E_{i,n}}}$$

$$Z \rightarrow Z' = A \cdot Z$$

$$ln(Z') = ln(Z) + ln(A)$$

- Keeping one value fixed reduces dimension

$$\Delta ln(Z_l) = 0$$

References

[1] M. E. J. Newman and G. T. Barkema, "Analysing Monte Carlo Data," in Monte Carlo Methods in Statistical Physics (M. E. J. Newman and G. T. Barkema, eds.), p. 0, Oxford University Press, Feb. 1999.

[2] A. M. Ferrenberg and R. H. Swendsen, "New Monte Carlo technique for studying phase transitions," Physical Review Letters, vol. 61, pp. 2635–2638, Dec. 1988. Publisher: American Physical Society.

[3] A. M. Ferrenberg and R. H. Swendsen, "Optimized Monte Carlo data analysis," Physical Review Letters, vol. 63, pp. 1195–1198, Sept. 1989. Publisher: American Physical Society.

[4] J. Raphson, Analysis aequationum universalis seu ad aequationes algebraicas resolvendas methodus generalis, & expedita, ex nova infinitarum serierum methodo, deducta ac demonstrata : ; cui annexum est de spatio reali, seu ente infinito conamen mathematico-metaphysicum / authore Josepho Raphson. 1697.

[5] T. J. Ypma, "Historical Development of the Newton-Raphson Method," SIAM Review, vol. 37, no. 4, pp. 531–551, 1995. Publisher: Society for Industrial and Applied Mathematics