Reweighting

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(Late) Summer School on Monte Carlo Methods

For concreteness, let us consider a Monte Carlo simulation of 2D Ising model at the critical coupling $\beta_c = \frac{1}{2}\log(1+\sqrt{2}) \approx 0.44$. MC simulation gives us a series of configurations $\Phi_1, \Phi_2 \ldots \Phi_N$, and measurements of some observable $O_i = O(\Phi_i)$.

Estimate of the expectation value:

$$\langle O \rangle_{\beta_c} \equiv \frac{1}{Z} \sum_{\{s\}} O(s)\, e^{-\beta_c E(s)} \approx \frac{1}{N} \sum_i O_i$$

Reweighting allows us to estimate $\langle O \rangle_\beta$, if $|\beta - \beta_c|$ is sufficiently small.

Basic principle: consider measurements O_i, E_i. Now

$$\frac{1}{N} \sum_i O_i e^{-(\beta-\beta_c)E_i} = \frac{\sum_{\{s\}} [O e^{-(\beta-\beta_c)E}]\, e^{-\beta_c E}}{Z_{\beta_c}}$$

$$\frac{1}{N} \sum_i e^{-(\beta-\beta_c)E_i} = \frac{\sum_{\{s\}} [e^{-(\beta-\beta_c)E}]\, e^{-\beta_c E}}{Z_{\beta_c}} = \frac{Z_\beta}{Z_{\beta_c}}$$

$$\mapsto \quad \boxed{\langle O \rangle_\beta = \frac{\sum_i O_i\, e^{-(\beta-\beta_c)E_i}}{\sum_i e^{-(\beta-\beta_c)E_i}}}$$

Note: $\sum_i$ goes over measurements, E_i, O_i must be measured from the same configuration.

In practice: during a MC run, write down all measurements E_i and various O_i in a file. After the run, use eq. $\square$ to calculate $\langle O \rangle_\beta$.

Alternative view (original method): reweighting using histograms (probability distributions)

- During a MC run (at β_c), measure histogram $h_{\beta_c}(E)$.
- We know that $h_\beta(E) \propto n(E) \exp(-\beta E)$, where $n(E)$ is the number of states at energy E.
- Thus, we can reweight h: $h_\beta(E) \propto h_{\beta_c}(E) \exp[-(\beta - \beta_c)E]$.
- Finally, if $O(E)$ is a function of energy, we can calculate

$$\langle O \rangle_\beta = \frac{\sum_E O(E) h_\beta(E)}{\sum_E h_\beta(E)} = \frac{\sum_E O(E) h_{\beta_c}(E) \exp[-(\beta - \beta_c)E]}{\sum_E h_{\beta_c}(E) \exp[-(\beta - \beta_c)E]}$$

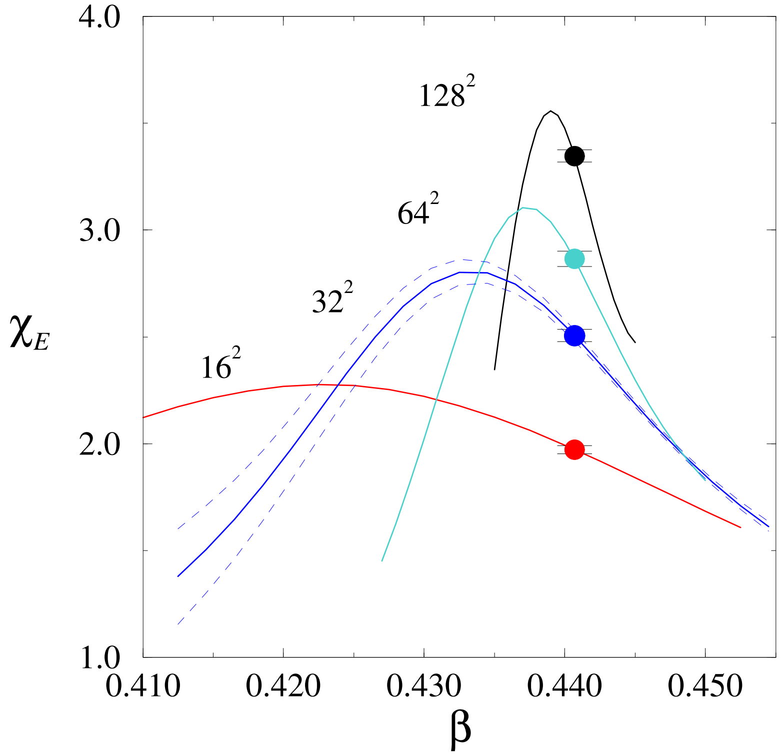
This works only if $O[\{s\}] = O[E(\{s\})]$ is a function of energy, whereas $\square$ works for arbitrary observable.
(histogram method can be obtained from $\square$ using $O = \delta_{E,E'}$.)

History:
- First proposed in '59 [Salzburg et al, J.Chem.Phys 30 (1959) 60]
- First used by McDonald and Singer 1967, no success (reweighting range too small?)
- Shown to be very effective by Ferrenberg and Swendsen [PRL 61 (1988) 2635]
- Multihistogram method: F+S [PRL 63 (1989) 1195; Computers in Physics, Sep/Oct 1988]

Example: 2d Ising, $V = 16^2 \dots 128^2$. Energy susceptibility (Heat capacity)

$$\chi_E = -\frac{1}{V}\frac{\partial\langle E\rangle}{\partial\beta} = \frac{1}{V}\langle(E-\langle E\rangle)^2\rangle$$

Susceptibility diverges with a critical exponent $\chi_E \sim L^{\alpha/nu}$ when $L \to \infty$ and we are at $\beta = \beta_c$:

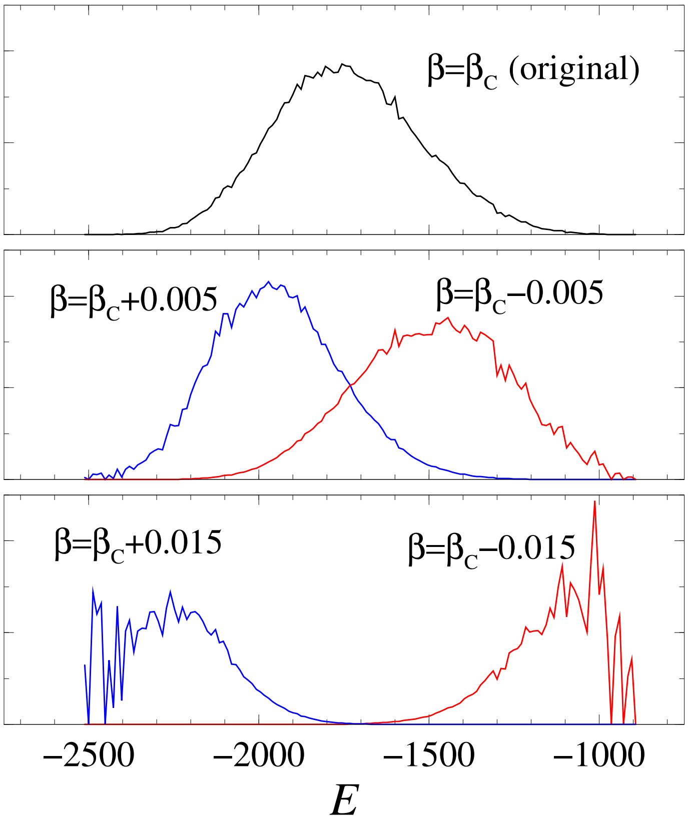


Points: simulated values, curves: reweighted data. Dashed lines show the error band for 32^2 (for clarity, not shown for others).

Errors analyzed here using jackknife. Use of jackknife or bootstrap methods strongly recommended!

Errors increase when reweighting distance increases. Must not do reweighting too far from original simulation point!

Energy histograms, 64^2 (probability distributions of E). Original simulation at $\beta = \beta_c \approx 0.44$.



The histograms become exponentially worse when the reweighting range increases.

How far one can reweight? Valid reweighting range $\ll$ 'fluctuation' range:

- **Simulation at non-critical point: $\Delta\beta \propto 1/\sqrt{V}$.**
- **At a critical point (as in our example): $\Delta\beta \propto 1/L^x$, where x is some critical exponent. In our case above, $x = d - \alpha/\nu$ (I think), where $d = 2$ is the dimensionality.**

PRAGMATIC VIEW: check that the 'mass' of the reweighted histogram does not shift too far away into tails of the original histogram, where there is insufficient amount of data!

Reweighting with respect to external magnetic field h: Ising model

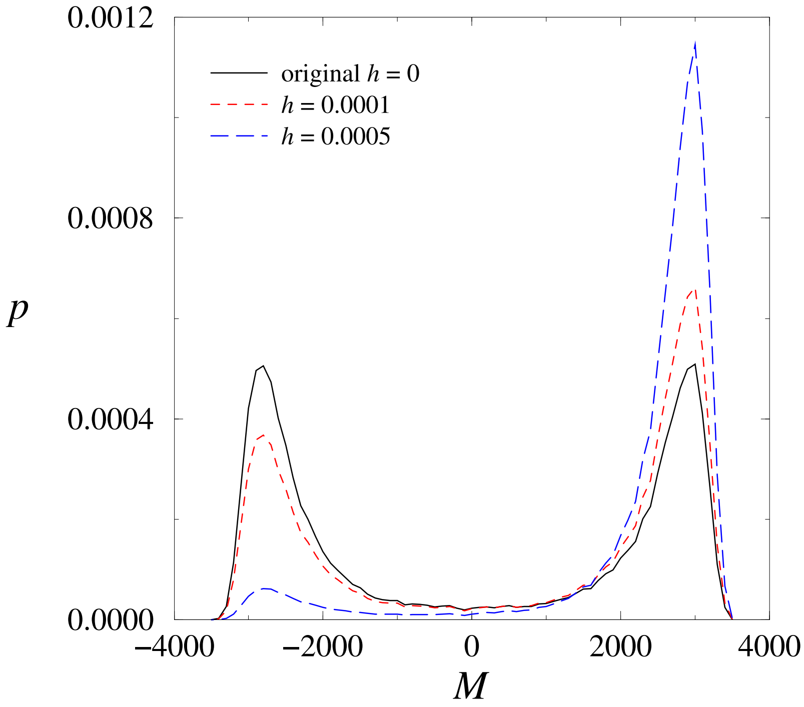
$$Z_{\beta,h} = \sum_s \exp[-\beta E + hM] \quad \textbf{where} \quad M = \sum_i s_i$$

If the original simulation was performed with h_s, reweighting in h is completely analogous to eq.$\square$:

$$\langle O \rangle_h = \frac{\sum_i O_i \, e^{(h-h_s)M_i}}{\sum_i e^{(h-h_s)M_i}}$$

Thus, even if originally $h_s = 0$ (no field in the original simulation), we can reweight to finite external field!

Magnetization histogram $p(M)$, size 64^2, in simulation $h = 0$, and $\beta = \beta_c$



Reweighting can be done simultaneously in β and h. (How? And why the original histogram reweighting is not practical in this case?)

Reweighting wrt. arbitrary parameters g^a, which couple to observables G^a: the partition function is

$$Z_g = \sum_s \exp[\sum_a g^a G^a]$$

Simulation is performed with $g^a = g^a_s$. Reweighting:

$$\langle O \rangle_g = \frac{\Sigma_i \, O_i \, \exp[\Sigma_a (g^a - g^a_s) G^a_i]}{\Sigma_i \exp[\Sigma_a (g^a - g^a_s) G^a_i]}$$

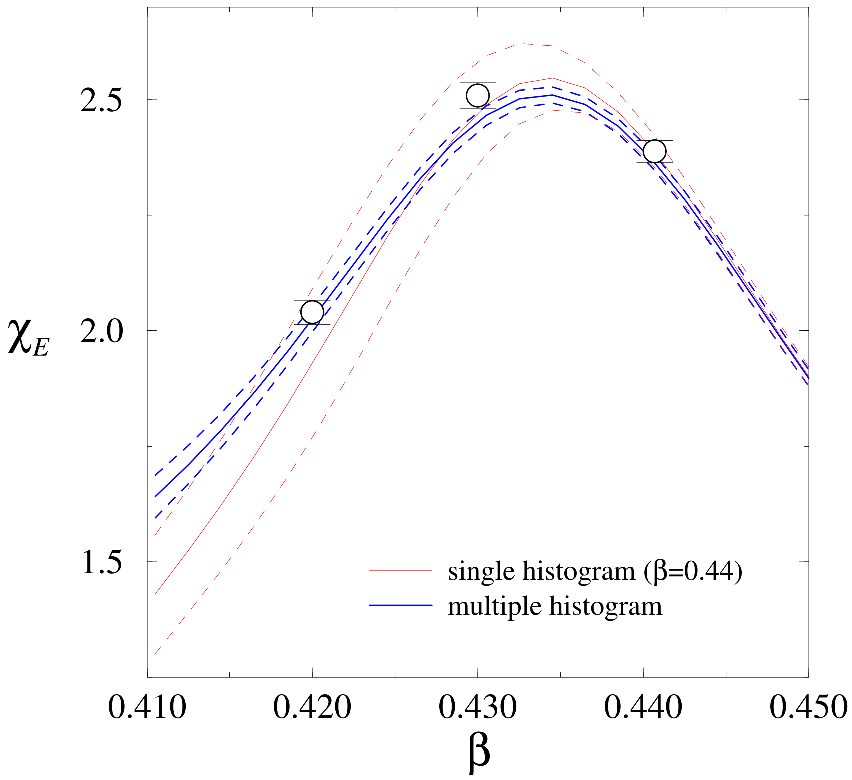
Thus, $g^1 = -\beta$, $G^1 = E$ recovers standard reweighting.

Finding Lee-Yang zeroes of the partition function: reweight to complex β, so that $Z_\beta = 0$.

Multiple histogram reweighting

Multiple histogram method joins together several sets of data, run at different β-values, in an optimized way.

Example:
Susceptibility χ_E, volume 32^2. The data from 3 runs is joined together with multiple histogram reweighting (blue curve). Errors are much smaller than with single histogram reweighting.



Powerful method – should be part of standard toolbox for everybody who can join points from different simulations. However, somewhat cumbersome to use.

- Perform R Monte Carlo simulations, at couplings β_i, with length N_i.
- Measure the energy distributions $p_i(E) = H_i(E)/N_i$, and the autocorrelation time τ_i.
- True distribution is given by

$$p_i(E) = n(E)\, e^{-\beta_i E + f_i},$$

where $n(E)$ is the density of states (does not depend on β), and f_i is (dimensionless) free energy: $f_i = -\log Z_{\beta_i}$.

$\mapsto$ Each of the simulations gives us an estimate of $n(E) = p_i(E)e^{\beta_i E - f_i}$ (we don't know f_i, so that the normalization is unknown). Since the MC runs were performed at different β_i, each of the run yields a reliable estimate of $n(E)$ only at limited range of E.

- **Optimization:** we obtain an improved estimate for $n(E)$ by combining all runs together:

$$n(E) = \sum_{i=1}^{R} r_i(E)p_i(E)e^{\beta_i E - f_i}, \quad \text{where} \quad \sum_{i=1}^{R} r_i(E) = 1 \quad \text{for all } E.$$

Note that the relative weights $r_i(E)$ are independent at each E: $\rightarrow$ optimization.

- $r_i(E)$ are determined by minimizing the (error)^2 in $n(E)$ (now follows somewhat technical derivation):
  - What is the uncertainty in histogram values? Assuming that $H_i(E)$ is Poisson distributed around the 'true' value $\bar{H}_i(E)$, we obtain

$$\delta^2 H_i(E) = g_i \bar{H}_i(E) = g_i N_i n(E) e^{-\beta_i E - f}\,.$$

    Here $g_i = 1 + 2\tau_i$ takes into account the autocorrelations in run i.
  - Thus, (error)^2 in $n(E)$

$$\delta^2 n(E) = \sum_i r_i^2(E) \frac{\delta^2 H_i(E)}{N_i^2} e^{2(\beta_i E - f_i)} = \sum_i r_i^2(E) \frac{g_i n(E)}{N_i} e^{\beta_i E - f_i}$$

– Minimize $\delta^2 n(E)$ wrt. $r_i(E)$ with condition $C \equiv \sum_i r_i(E) = 1$. Use Lagrange multipliers (try it):

$$\frac{\partial}{\partial r_i(E)}[\delta^2 n(E) + \lambda C] = 0 \quad \mapsto \quad r_i(E) = \frac{N_i g_i^{-1} e^{-\beta_i E + f_i}}{\sum_{j=1}^R N_j g_j^{-1} e^{-\beta_j E + f_j}}$$

- Thus, the optimized expression for $n(E)$ is

$$n(E) = \frac{\sum_{i=1}^R g_i^{-1} H_i(E)}{\sum_{j=1}^R N_j g_j^{-1} e^{-\beta_j E + f_j}}$$

- The coefficients f_i are then determined by solving

$$e^{-f_i} = \sum_E n(E) e^{-\beta_i E}$$

  To solve this equation use some iterative method (Newton-Raphson). f_i's are determined up to an additional constant.

- Observable expectation values:

$$\langle O \rangle_\beta = \frac{\sum_E O(E) n(E) e^{-\beta E}}{\sum_E n(E) e^{-\beta E}}$$

As with the single histogram method, this can be formulated without resorting to $H_i(E)$. Let E_i^a be the energy measurement number a ($a = 1 \ldots N_i$) from run number i. The expression for the free energy f_β becomes

$$e^{-f_\beta} = \sum_{i=1}^R \sum_{a=1}^{N_i} \frac{g_i^{-1} e^{-\beta E_i^a}}{\sum_{j=1}^R N_j g_j^{-1} e^{-\beta_j E_i^a + f_j}}.$$

f_i's are then solved from $e^{-f_i} = e^{-f_{\beta_i}}$, in analogy to the second eq. in the box above. The expectation value of O at reweighted β:

$$\langle O \rangle_\beta = \sum_{i=1}^R \sum_{a=1}^{N_i} \frac{O_i^a g_i^{-1} e^{-\beta E_i^a - f_\beta}}{\sum_{j=1}^R N_j g_j^{-1} e^{-\beta_j E_i^a + f_j}}$$