Lattice QCD - Fall 2017 ETH Zürich

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Exercise Nr. 11

Discussion on December 12th, 14:45

1) Single histogram reweighting

When studying phase transitions numerically we can only sample discrete points of some underlying (piecewise) continuous function of some external parameter, e.g. coupling or temperature. To reliably find maxima or intersections of these curves it would be desirable to sample them densely which, however, can be very time consuming. A better alternative is to interpolate between the sampled points (or to a lesser extent, extrapolate to nearby couplings). This can be done reliably if the important configurations at the sampled coupling overlaps with the important configurations of the target coupling. We can then *reweight* the configurations at one value of the coupling to obtain estimates for some observable O at another coupling. The easiest is to extrapolate around one sample, say at coupling β_0. The method is based on the following observation:

$$\langle O \rangle_\beta = \frac{1}{Z_\beta} \int \mathcal{D}[\phi] O(\phi) e^{-S_\beta(\phi)} = \frac{1}{Z_\beta} \int \mathcal{D}[\phi] O(\phi) e^{-(S_\beta(\phi) - S_{\beta_0}(\phi))} e^{-S_{\beta_0}(\phi)} = \frac{\left\langle O e^{-(S_\beta - S_{\beta_0})} \right\rangle_{\beta_0}}{\left\langle e^{-(S_\beta - S_{\beta_0})} \right\rangle_{\beta_0}}, \quad (1)$$

which expresses the observable at coupling β as a ratio of expectation values at β_0. Consider the Ising model for simplicity. Given N Monte Carlo measurements of (M_i, E_i) at inverse temperature β_0, where $M = \sum_i \sigma_i$ is the magnetization and $E = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j$ is the total energy, show that the magnetization at β is given by

$$\langle M \rangle_\beta = \left[\sum_{i=1}^{N} M_i e^{-(\beta - \beta_0)(E_i - \langle E \rangle)} \right] \left[\sum_{i=1}^{N} e^{-(\beta - \beta_0)(E_i - \langle E \rangle)} \right]^{-1}. \quad (2)$$

The shift by the mean energy $\langle E \rangle$ is arbitrary but convenient for numerical purposes. Simulate the square $2d$ Ising model at $\beta_0 = \beta_c = \log(1 + \sqrt{2})/2$ and measure the energy per spin, $\langle U \rangle = \langle E \rangle / L^2$, and the specific heat per spin, $\langle C \rangle = L^2 \beta^2 (\langle U^2 \rangle - \langle U \rangle^2)$, and reweight to $\beta \in [0.3, 0.6]$. Compare with the exact results for an $L \times L$ lattice [1]. Try to come up with a condition for the reliability of the reweighting. Hint: assume configurations which are Gaussian as a function of the energy and consider the overlap at different β.

[1] A. E. Ferdinand and M. E. Fisher Phys. Rev. **185** (1969) 832.

2) Multi-histogram reweighting

Multi-histogram was proposed by Salzburg et al [2] but first successfully used by Ferrenberg and Swendsen [3] and now goes under the name F-S reweighting. It is motivated by the fact that interpolation is more reliable than extrapolation. The basic idea is to perform Monte Carlo simulations at a few (not to sparsely separated) couplings and use the information to interpolate to couplings in-between. To derive the formula, let us first note that the single histogram can be formulated in terms of energy histograms $h_\beta(E) \propto n(E)e^{-\beta E}$ where $n(E)$ is the number of states at energy E. This leads to

$$\langle O \rangle_\beta = \frac{\sum_E O(E)h_\beta(E)}{\sum_E h_\beta(E)} = \frac{\sum_E O(E)h_{\beta_0}(E)e^{-(\beta-\beta_0)E}}{\sum_E h_{\beta_0}(E)e^{-(\beta-\beta_0)E}}, \tag{3}$$

which is particularly useful if the possible energies are discrete. Consider now R Monte Carlo simulations at different couplings β_i, each with N_i measurements. Each of them has an energy distribution $h_i(E) = H_i(E)/N_i = n(E)e^{-\beta_i E+f_i}$, where f_i is the free energy. Since $n(E)$ is independent of β each measurement gives an estimate of it which can be combined to obtain an improved estimate:

$$n(E) = \sum_{i=1}^{R} r_i(E)h_i(E)e^{\beta_i E-f_i}, \text{ with } \sum_{i=1}^{R} r_i(E) = 1 \; \forall E. \tag{4}$$

Each simulation is only reliable in an energy range around where its histogram is peaked whence the weights $r_i(E)$ need to be optimized for each E. This is done by minimizing the square of the error in $n(E)$. Assuming a Poisson distribution of $H_i(E)$ around its true value $\bar{H}_i(E)$ we obtain

$$\delta^2 H_i(E) = g_i \bar{H}_i(E) = g_i N_i n(E) e^{-\beta_i E+f_i}, \; g_i = 1 + 2\tau_i, \tag{5}$$

where τ_i is the auto-correlation time of the energy in run i. The error in $n(E)$ can be expressed in terms of the error in $H_i(E)$:

$$\delta^2 n(E) = \sum_{i=1}^{R} r_i^2(E) \frac{\delta^2 H_i(E)}{N_i^2} e^{2(\beta_i E-f_i)} = \sum_{i=1}^{R} r_i^2(E) \frac{g_i n(E)}{N_i} e^{\beta_i E-f_i}. \tag{6}$$

Minimize this error with respect to $r_i(E)$ under the condition that $\sum_i r_i(E) = 1$ to obtain

$$n(E) = \sum_{i=1}^{R} g_i^{-1} H_i(E) \left[\sum_{j=1}^{R} N_j g_j^{-1} e^{-\beta_j E+f_j} \right]^{-1}, \quad e^{-f_i} = \sum_E n(E)e^{-\beta_i E}. \tag{7}$$

Since the free energies enters in $n(E)$ these equations have to be solved iteratively. After $n(E)$ has been determined we can reweight our observables:

$$\langle O \rangle_\beta = \frac{\sum_E O(E)n(E)e^{-\beta E}}{\sum_E n(E)e^{-\beta E}}. \tag{8}$$

However, it is usually not practical to measure the energy histograms. Show that eqs.(7- 8) can be brought to the form

$$e^{-f_\beta} = \sum_{i=1}^{R} \sum_{a=1}^{N_i} \left[\sum_{j=1}^{R} N_j \frac{g_i}{g_j} e^{-(\beta_j-\beta)(E_i^a-\langle E \rangle)+f_j} \right]^{-1}, \; \langle O \rangle_\beta = \sum_{i=1}^{R} \sum_{a=1}^{N_i} O_i^a \left[\sum_{j=1}^{R} N_j \frac{g_i}{g_j} e^{-(\beta_j-\beta)(E_i^a-\langle E \rangle)+f_j-f_\beta} \right]^{-1}, \tag{9}$$

with self-consistency condition $f_i = f_{\beta_i}$. Add two or three measurements in the interval in **1)** and perform a F-S reweighting in the same interval.

[2] Salzburg et al J. Chem. Phys. **30** (1959) 60.
[3] A. M. Ferrenberg and R. H. Swendsen Phys. Rev. Lett. **61** (1988) 2635.

3) Jackknife error analysis

It is not entirely straightforward to obtain reliable errors on the reweighted observable. One option is to do a Jackknife [4,5] or Bootstrap [5] analysis on the data. We will here only treat the Jackknife. Both methods *resample* the existing data to obtain new data sets to perform the error analysis on. Simply put, the Jackknife measures the impact of removing a portion of the data and produces an estimate of the error based on this. More precise, consider some function f which depends on some observables $\vec{O}$ contained in some date set $\{\vec{O}_i\}_{i=1}^N$. The first step is to get rid of auto-correlations, this is done by binning the data in M bins of length $\gg \tau$. We then proceed to calculate the $f_{(m)}$ on the data set where bin m is *removed*. From this set of values we can calculate the Jackknife error,

$$\delta\hat{f} = \sqrt{\frac{M-1}{M}\sum_{m=1}^{M}\left(\left\langle f_{(m)}\right\rangle - \left\langle \hat{f}\right\rangle\right)^2}, \tag{10}$$

where $\left\langle \hat{f}\right\rangle = \sum_m \left\langle f_{(m)}\right\rangle /M$. In the case of a simple observable, for example $f = \langle O\rangle$, this reduces to the standard (binned) error estimate

$$\delta O = \sqrt{\frac{\sum_{m=1}^{M}(\langle O_m\rangle - \langle O\rangle)^2}{M(M-1)}} \tag{11}$$

but the main application is to estimate the errors of observables which depends on the complete data set like reweighted observables or correlations where we cannot directly construct a time series to measure the standard deviation of. Implement the Jackknife algorithm and include errorbars for your reweighted observables in **1)** and **2)**.

[4] R. G. Miller, "The jackknife - a review", Biometrika **61** (1971) pg. 1-17.
[5] B. Efron, "The Jackknife, the Bootstrap and Other Resampling Plans", Society for Industrial and Applied Mathematics (1982)