KFU Graz

Dénes Sexty (denes.sexty@uni-graz.at)

CP1: Monte Carlo Methods WS 2023/24

16. Exercise: Reweighting the Ising model

In this exercise we look at reweighting the 3d Ising model to different temperatures. The action is

$$H = -J\sum_{neigh} s_i s_j - h\sum_i s_i, \quad M = \frac{1}{N^3}\sum_i s_i$$
 (1)

on a periodic N^3 lattice. You can find a file called <code>ising3d_N16_magnabsavr.dat</code> on the moodle page which contains the average magnetization and its error (2nd and 3rd column) as a function of the J parameter (1st column) as measured by some MC simulations at h=0 and N=16.

On the moodle page you also find a datafile magnabs_actdens_ising3d_N16_J0.21.dat which contains the absolute value of the magnetisation and the action density (without the J factor so $H/(JN^3)$ in the notation above) for configurations in an MC simulation of the Ising model at h=0, N=16, J=0.21 (one configuration per line, first column is magnetization, second is action density).

Now we want to reweight the measurements at J=0.21 to other J values. As discussed on the lecture, we use the following formula:

$$\langle M \rangle_J = \frac{\sum M_c w_c}{\sum w_c} = \frac{\sum M_c w_c \frac{w'_c}{w'_c}}{\sum w_c \frac{w'_c}{w'_c}} = \frac{\langle M w / w' \rangle_{J'}}{\langle w / w' \rangle_{J'}}$$
(2)

with c indexing the possible spin configurations of the Ising model and the Boltzman factor $w_c = \exp(-JH_c)$ and the Boltzmann factor at J': $w'_c = \exp(-J'H_c)$.

- Take the starting ensemble at J=0.21 and reweight it in steps of $\Delta J=0.01$ to a different J' in decreasing as well as increasing directions. Compare your results to the results of simulations at those J values (which you can take from the first datafile). What do you notice? (Here you might run into a technical problem because $\exp(-\Delta Ja*16^3)$, with the average action density a, might be too small/large in magnitude to be represented by your computer. To solve this problem note that the you can add a constant to the action without changing the physics of the system).
- Calculate jackknife errors (use jackknife_mclect.py, and compare with the direct simulations. How do you interpret your findings? (Hint: look at the distribution of the reweighting factors)
- There seems to be a difference in reweighting to smaller and larger values of J regarding e.g. the statistical errors one gets. What could be the physical reason for that?