2009
Computer Exercises
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Session 3 : Advanced Monte-Carlo techniques

1 Multiple-histogram reweighting

We apply the method to $2D$-Ising model. The multiple-histogram method consists of collecting all the information from several importance sampling runs at different temperatures. Assume that we generated r runs at temperatures $\{T_i\}$. From each run, we stored the histogram $\mathcal{N}_i(M, NNC)$. The probability to observe (M, NNC) is then given by

$$p_i(M, NNC) = \frac{\mathcal{N}_i(M, NNC)}{\mathcal{N}_i^{tot}} = \frac{D(M, NNC)\exp(-\beta_i E(M, NNC))}{Z_i} \tag{1}$$

By inverting Eq.(1), we find an estimation of D, and then, for an arbitrary temperature, the estimated probability to observe (M, NNC) is

$$p_i^{est,T}(M, NNC) = p_i(M, NNC)\frac{Z_i}{Z}\exp\left((\beta_i - \beta)E(M, NNC)\right) \tag{2}$$

We want to combine all the $p_i^{est,T}$ into an improved estimation of p^T

$$p^{est,T} = \sum_{i=1}^{r} w_i p_i^{est,T} \tag{3}$$

with $\sum_i w_i = 1$ and $w_i \geq 0$. What is the best choice for the weights? The minimization of the estimated error of $p^{est,T}$ gives the optimal choice

$$w_i = \frac{1/\sigma^2_{p_i^{est,T}}}{\sum_{j=1}^{r} 1/\sigma^2_{p_j^{est,T}}} \tag{4}$$

Each individual bins of p_i follows a Poisson distribution. Therefore, one can show that

$$\sigma^2_{p_i} = \frac{p_i}{\mathcal{N}_i^{tot}} \tag{5}$$

and then,

$$\sigma^2_{p_i^{est,T}} = \frac{p^{est}}{\mathcal{N}_i^{tot}}\frac{Z_i}{Z}\frac{\exp(-\beta E)}{\exp(-\beta_i E)} \tag{6}$$

Finally, with Eqs.(3), (4) and (6),we find

$$p^{est,T}(M, NNC) = \frac{\sum_{i=1}^{r}\mathcal{N}_i(M, NNC)}{\sum_{i=1}^{r}\mathcal{N}_i^{tot}\frac{Z}{Z_i}\exp\left((\beta - \beta_i)E(M, NNC)\right)} \tag{7}$$

1. The last step is to determine the Z_i. Show that they verify the self-consistent equations

$$Z_i = \sum_{(M,NNC)}\left(\frac{\sum_{j=1}^{r}\mathcal{N}_j(M, NNC)}{\sum_{j=1}^{r}\mathcal{N}_j^{tot}\frac{\exp(-\beta_j E(M,NNC))}{Z_j}}\right)\exp(-\beta_i E(M, NNC)) \tag{8}$$

2. How can one solve the preceding system of equations?
3. Complete the subroutine *equation.f90* to compute the Z_i.
4. Complete the subroutine *density.f90* to evaluate the density of state.
5. With $\{T_i = 1.5, 2, 2.5, 3, 4, 5, 6, 8, 10\}$, compute the corresponding evolution of $\bar{M}(T)$ with the multiple-histogram method. Compare with simple and importance sampling.
6. Code a subroutine to compute the heat capacity. Compute $C_v(T)$ and estimate the critical temperature.

2 Multicanonical reweighting

We apply the method to $2D$-Ising model. This method belongs to the family of biaised algorithms (like the Rosenbluth sampling). The point is to make a walk in the configuration space according to a given distribution $\pi(M, NNC)$ using spin flips (like in importance sampling). It means that the histogram of the visited configurations $\mathcal{N}_\pi(M, NNC)$ has to be proportionnal to $D(M, NNC) \times \pi(M, NNC)$.

1. Why can importance sampling be viewed as a particular case of this method? For which π?
2. Derive an acceptance rule (similar to the Metropolis criterion) for an arbitrary distribution π.
3. For each configuration, we assign a weight $W_i(T) = \exp(-\beta E_i)/\pi_i$. Proove that $\langle X\rangle(T) = \sum_i X_i W_i / \sum_i W_i$.
4. Complete the subroutine *walk.f90* to code the acceptance rule and compute $\mathcal{N}_\pi(M, NNC)$.
5. Complete the subroutine *density.f90* to compute the corrected density of state from $\mathcal{N}_\pi(M, NNC)$.
6. First, take $\pi = 1$. Plot the resulting histogram. Any comments?
7. Now, for π take the estimation of the density of state computed with simple sampling. What do you except to find for $\mathcal{N}_\pi$? Compare with the computed results and trace $\bar{M}(T)$. Any comments?
8. Complete the *maincano.f90* program to iteratively converge to the correct density of state.