2009
Computer Exercises
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Session 3 : Advanced Monte-Carlo techniques - correction

1 Multiple-histogram reweighting

1. With $Z_i = \sum_{(M,NNC)} D(M,NNC)\exp(-\beta_i E)$, $D = Z\exp(\beta E)p^{est,T}$ and $p^{est,T}$ given by Eq.(7).
2. Eq.(8) could be rewritten $\vec{Z} = \vec{f}(\vec{Z})$ where $\vec{Z} = (Z_1, ..., Z_r)$ and $\vec{f}$ a vectorial function. We can solve Eq.(8) by finding the limit of the serie $\vec{Z}_{n+1} = \vec{f}(\vec{Z}_n)$ for an arbitrary initial condition.
3. see the corrected code.
4. see the corrected code.
5. see Fig.1

2 Multicanonical reweighting

1. Importance sampling makes a walk in the configuration space according to the Boltzmann distribution. So if $\pi = \exp(-\beta E)$, we recover the importance sampling method.
2. We want to sample the π-ensemble at equilibrium. Then, the detailed balance imposes that the number of transition from any state o to any state n is equal to the number of transition from n to o: $N(o \to n) = N(n \to o)$. We can decompose $N(o \to n) = \mathcal{N}(o)\alpha(o \to n)accep(o \to n)$ where $\mathcal{N}(o)$ number of state in o at equilibrium, $\alpha(o \to n)$ the probability to construct a move from o to n, and $accep(o \to n)$ the probability to accept the move. It gives

$$\mathcal{N}(o)\alpha(o \to n)accep(o \to n) = \mathcal{N}(n)\alpha(n \to o)accep(n \to o) \tag{1}$$

   α is assumed symmetric then

$$\frac{accep(o \to n)}{accep(n \to o)} = \frac{\mathcal{N}(n)}{\mathcal{N}(o)} = \frac{\pi(n)}{\pi(o)} \tag{2}$$

   Then, we take the Metropolis choice: $accep(o \to n) = min(1, \pi(n)/\pi(o))$.
3. $\sum_i X_i W_i = \sum_{(M,NNC)} \mathcal{N}_\pi(M,NNC)X(M,NNC)\exp(-\beta E(M,NNC))/\pi(M,NNC)$
   $= \sum_{(M,NNC)} D(M,NNC)X(M,NNC)\exp(-\beta E(M,NNC))$ + Idem for $\sum_i W_i$.
4. see the corrected code.
5. see the corrected code.
6. With $\pi = 1$, the method is equivalent to simple sampling.
7. If $\pi = 1/D$, the histogram has to be flat. However, with simple sampling, we have a bad estimation of D so $\mathcal{N}_\pi$ is flat only around the center of the distribution.

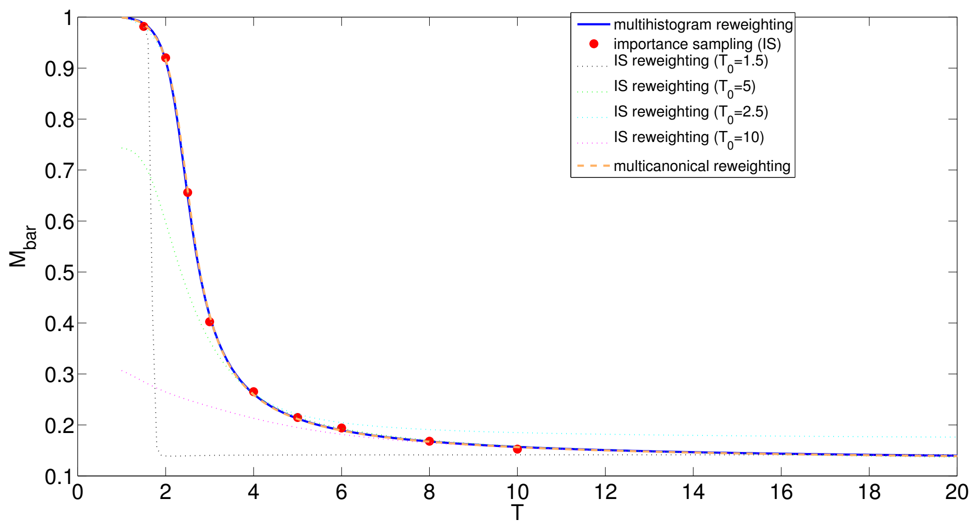

Figure 1: $\bar{M}$ computed with different methods.

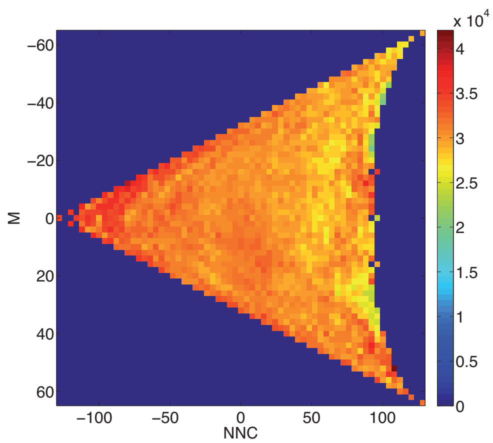

Figure 2: Final histogram of the iterative process

8. By iteratively using the inverse of the computing D as an input of the program, we quickly converge to the "good" density of state and the final histogram is nearly flat (6-7 iterations are enough), see Fig.2.