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Computer Exercises
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Session 2 : importance and Rosenbluth sampling - correction

1 $2D$-Ising model

1. From a initial random matrix, we iteratively change the configuration and we accept the new config with a probability $\min(\exp(-\beta\Delta E), 1)$ with $\Delta E = E(n) - E(o)$ (Metropolis criterion). If the differences between the old and new configurations are too important, ΔE is more likely to be highly positive and the new config will be more rejected. That's why it is better to make local moves like spin flips.
   For a spin flip at position (i, j), $\Delta E = -2S(i,j)(S(i+1,j) + S(i,j+1) + S(i-1,j) + S(i+1,j))$

2. The histogram reflects the canonical distribution, therefore, we need to update $\mathcal{N}_0(M, NNC)$ even if a configuration is rejected.
   $\langle X\rangle(T_0) = (\sum_i X(M_i, NNC_i))/N_f = (\sum_{M,NNC} X(M, NNC)\mathcal{N}_0(M, NNC))/(\sum_{M,NNC} \mathcal{N}_0(M, NNC))$.

3. $\sigma^2_{\langle X\rangle} = 1/N_f^2 \times \sigma^2_{\sum_i X_i}$. We can decompose the sum_i into a sum over N_b independent blocks: $\sum_i X_i = \sum_{k=1}^{N_b}(\sum_{i=1}^{N_f/N_b} X_i) = N_f/N_b \sum_{k=1}^{N_b} \tilde{X}_k$ with $\tilde{X}_k = N_b/N_f \sum_{i=1}^{N_f/N_b} X_i$ the average value of X within a correlated block. N_f/N_b represents the typical decorrelation length. Then, $\sigma^2_{\sum_i X_i} = (N_f/N_b)^2 \times N_b \times \sigma^2_{\tilde{X}}$. So, $\sigma^2_{\langle X\rangle} = \sigma^2_{\tilde{X}}/N_b$.

4. see the corrected code.

5. see the corrected code.

6. $\mathcal{N}_0(M, NNC) \sim D(M, NNC)\exp(NNC/T_0)$. So, the density of state is proportional to $\mathcal{N}_0(M, NNC)\times \exp(-NNC/T_0)$.

7. see the corrected code.

8. During the MC process, we generate states which are relevant at T_0. That's why the computed behavior of $\bar{M}(T)$ is confident for T closed to T_0. At $T_0 = T_c$, fluctuations of the system are important, and the system visits a widespread number of states. That's why the best results are given by the run at T_c.

9. For all T, the histogram is nearly symmetric in M. After T_c, the net magnetization is null and the histogram is picked around $M = 0$. Before T_c, the magnetization is non-zero and the histogram has two peacks around $M = \pm|M_T|$. At T_c, the histogram is flat around $M = 0$. For 8×8 system, we found $T_c = 2.83 \pm 0.01$.

2 Rosenbluth sampling for chain molecules

2.1 The method

1. If we follow the Rosenbluth scheme, the probability to generate a given conformation is $P(\Gamma) = \prod_{i=1}^{N+1} p^i(l) = \exp(-\beta U(\Gamma))/W(\Gamma)$. Then, $(\sum_i W_i X_i)/(\sum_i W_i) = (\sum_\Gamma W(\Gamma)X(\Gamma)P(\Gamma))/(\sum_\Gamma W(\Gamma)P(\Gamma)) = (\sum_\Gamma X(\Gamma)\exp(-\beta U(\Gamma)))/(\sum_\Gamma \exp(-\beta U(\Gamma)) = \langle X\rangle$.

2. $\sigma^2_{\langle X\rangle} = \sigma^2_{\sum_{i=1}^M W_i X_i}/(M^2\langle W\rangle^2)$. If we assume that W and X are independent variables: $\sigma^2_{\langle X\rangle} = \langle W^2\rangle/\langle W\rangle^2\sigma^2_X/M$.

3. $\langle W\rangle = 1/M \sum_i W_i = \sum_\Gamma P(\Gamma)W(\Gamma) = \sum_\Gamma \exp(-\beta U(\Gamma)) = Z$.

4. The Rosenbluth scheme is a static method (two different sequences are generated independently from each other) (compared to the dynamic importance sampling of Exercise 1). It is also a biased sampling.

2.2 Application to $3D$ SAW

We apply the Rosenbluth technique to $3D$ SAW.

1. see the corrected code.
2. see the corrected code.
3. $c = 0.588$ and $\mu = 4.68$.
4. The method fails for long sequences. In fact, one a show that the Rosenbluth sampling tends to generate compact structures with small weight. Relevant conformations (with high W) are not sampled.