Lattice QCD - Fall 2017 ETH Zürich

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Exercise Nr. 7

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1) Autocorrelation time

In a Monte Carlo simulation, we have

$$\langle \mathcal{O} \rangle \;=\; \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}_i, \tag{1}$$

where $\mathcal{O}_i$ is the value of the observable $\mathcal{O}$ obtained on the i-th configuration of the Markov chain. The true expectation value $\langle \mathcal{O} \rangle$ would be an ordinary number, but for finite length N of the Markov chain, its estimator,

$$\overline{\mathcal{O}} \;=\; \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}_i \tag{2}$$

is in fact a random variable, fluctuating around $\langle \mathcal{O} \rangle$. Therefore, in order to derive any conclusion from a simulation, we should in addition to $\overline{\mathcal{O}}$ also determine its statistical error $\epsilon_{\overline{\mathcal{O}}} \;=\; \sqrt{\sigma^2_{\overline{\mathcal{O}}}}$, where

$$\sigma^2_{\overline{\mathcal{O}}} \;=\; \left\langle \overline{\mathcal{O}}^2 \right\rangle - \left\langle \overline{\mathcal{O}} \right\rangle^2, \tag{3}$$

which, using (2) reads,

$$\sigma^2_{\overline{\mathcal{O}}} \;=\; \frac{1}{N^2} \sum_{i,j=1}^{N} \left(\langle \mathcal{O}_i \mathcal{O}_j \rangle \;-\; \langle \mathcal{O}_i \rangle \langle \mathcal{O}_j \rangle \right) \tag{4}$$

$$\;=\; \frac{1}{N^2} \sum_{i=1}^{N} \underbrace{\left(\langle \mathcal{O}_i \mathcal{O}_i \rangle \;-\; \langle \mathcal{O}_i \rangle \langle \mathcal{O}_i \rangle \right)}_{\sigma^2_{\mathcal{O}_i}} + \frac{1}{N^2} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} \left(\langle \mathcal{O}_i \mathcal{O}_j \rangle \;-\; \langle \mathcal{O}_i \rangle \langle \mathcal{O}_j \rangle \right). \tag{5}$$

The straight forward way to estimate (5) would be to use values of $\mathcal{O}_i$ obtained by performing the same simulation many times. In this case the second sum on the second line of (5) would vanish as the values $\mathcal{O}_i$ obtained from the i-th configurations of independent Markov chains would be statistically independent, i.e. $\langle \mathcal{O}_i \mathcal{O}_j \rangle \;=\; \langle \mathcal{O}_i \rangle \, \langle \mathcal{O}_j \rangle$ for $i \neq j$ and we would just have

$$\sigma^2_{\overline{\mathcal{O}}} \;=\; \sigma^2_{\mathcal{O}_i} / N, \tag{6}$$

as $\sigma^2_{\mathcal{O}_i}$ should be the same for all i.
Running the same simulation many times is of course highly unpractical and we would like to estimate (5) from just a single simulation. To do so, we can again approximate all expectation values appearing in (5) by the corresponding estimators obtained from a single Markov chain $\left\langle \mathcal{O} \right\rangle \;\approx\; 1/M \, \sum_{i=1}^{M} \mathcal{O}_i$. Equation (5) then becomes

$$\sigma^2_{\overline{\mathcal{O}}} \;\approx\; \frac{\sigma^2_{\mathcal{O}}}{N} \;+\; \frac{1}{N^2} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} \left(\mathcal{O}_i \mathcal{O}_j \;-\; \overline{\mathcal{O}}^2 \right) \;=\; \frac{\sigma^2_{\mathcal{O}}}{N} \;+\; \frac{2}{N^2} \sum_{j=1}^{N-1} \sum_{i=1}^{N-j} \left(\mathcal{O}_i \mathcal{O}_{i+j} \;-\; \overline{\mathcal{O}}^2 \right) \;=\; \frac{\sigma^2_{\mathcal{O}}}{N} \, 2 \, \tau^{int}_{\mathcal{O}}, \tag{7}$$

where $\sigma^2_{\mathcal{O}} = \frac{1}{N}\sum\limits_{i=1}^{N}\left(\mathcal{O}_i^2 - \overline{\mathcal{O}}^2\right)$, and where after the last equality sign, we have introduced the *integrated autocorrelation time* corresponding to the observable $\mathcal{O}$,

$$\tau^{int}_{\mathcal{O}} \;=\; \frac{1}{2} \;+\; \frac{\sum\limits_{j=1}^{N-1}\sum\limits_{i=1}^{N-j}\left(\mathcal{O}_i\mathcal{O}_{i+j} \;-\; \overline{\mathcal{O}}^2\right)}{\sum\limits_{i=1}^{N}\left(\mathcal{O}_i^2 - \overline{\mathcal{O}}^2\right)}. \tag{8}$$

Comparing (7) with expression (6), which would be the result if we used uncorrelated data to estimate $\sigma^2_{\overline{\mathcal{O}}}$, suggests that $N^{eff}_{\mathcal{O}} = N/\left(2\tau^{int}_{\mathcal{O}}\right)$ could be interpreted as the effective number of uncorrelated measurements of $\mathcal{O}$ in our Markov chain.

1. Write a program that uses data, produced by your 2d-Ising program, to measure the *running* integrated autocorrelation time for the energy density $h = H/V$ (where H, V are respectively the total energy and volume of the Ising system),

$$\tau^{run}_{h}\left(k\right) \;=\; \frac{1}{2} \;+\; \frac{\sum\limits_{j=1}^{k}\sum\limits_{i=1}^{N-j}\left(h_i\, h_{i+j} \;-\; \bar{h}^2\right)}{\sum\limits_{i=1}^{N}\left(h_i^2 - \bar{h}^2\right)} \tag{9}$$

   and outputs τ^{run}_h as a function of k. Then plot the result.

2. You should find that (9) becomes very noisy for large values of k. When computing (8), we must therefore find a compromise between the large statistical errors coming from these terms and the systematic error caused by dropping them. Usually one truncates the summation to $\tau^{int}_{\mathcal{O}} \approx \tau^{run}_{\mathcal{O}}\left(k^{max}\right)$ such that k^{max} is the smallest k satisfying $k > 6\,\tau^{run}_{\mathcal{O}}\left(k\right)$. The error can then be estimated as $\epsilon_{\tau^{int}_{\mathcal{O}}} \approx \tau^{int}_{\mathcal{O}}\sqrt{2\big(2k^{max}+1\big)/N} \approx \tau^{int}_{\mathcal{O}}\sqrt{12/N^{eff}}$. Implement this in your program.

3. Generate plots of τ^{int}_h (including error bars) as a function of the inverse temperature β for different system sizes $L \in \{10, 20, 30, 40, \ldots\}$.

4. Determine the scaling of $\tau^{int,pcr}_h = \tau^{int}_h\left(\beta^{pcr}\left(L\right), L\right)$ at the pseudo-critical point $\beta^{pcr}\left(L\right)$ as a function of the system size by using a power law ansatz $\tau^{int,pcr}_h = c\, L^z$.

5. Repeat the last two steps using data obtained with the cluster algorithm for the same set of simulation parameters and compare with the Metropolis case. What can you say about the magnitude and scaling behavior of the integrated autocorrelation time for the two algorithms?

2) Jack-knife method for error estimation

Using the autocorrelation time to compute reasonable error bars for observables is still very unpractical. Alternatives would be a *binning analysis* [1] or the so called *resampling methods* among which we will focus on the Jack-knife method as it has become the standard technique for estimating the errors of results obtained from Monte Carlo data.
The Jack-knife method works as follows: for a set $S = \{\mathcal{O}_1, \ldots, \mathcal{O}_N\}$ of N measuremetns of an observable $\mathcal{O}$ obtained by Monte Carlo simulation,

1. split S into M bins $b_i = \left\{\mathcal{O}_{(i-1)b+1}, \ldots, \mathcal{O}_{i\,b}\right\}$, $i \in \{1, \ldots, M\}$, such that $b = N/M >> 2\tau^{int}_{\mathcal{O}}$

2. define the i-th Jack-knife set as $\mathcal{O}_{(i)} = S \backslash b_i$

3. compute the means $\overline{\mathcal{O}} = \frac{1}{N}\sum_{i=1}^{N}\mathcal{O}_i$ and $\overline{\mathcal{O}}_{(j)} = \frac{1}{N-b}\sum_{i=1}^{N-b}\mathcal{O}_{(j),i}$ for all j

4. determine the Jack-knife error as: $\epsilon_{\mathcal{O}} = \sqrt{\frac{M-1}{M}\sum_{i=1}^{M}\left(\overline{\mathcal{O}}_{(i)} - \overline{\mathcal{O}}\right)^2}$

As we apriori don't know the autocorrelation time, we can measure the error $\epsilon_{\mathcal{O}}$ as a function of decreasing M. As soon as the error stops to increase when M is further decreased, M should be small enough such that $b = N/M >> 2\tau_{\mathcal{O}}^{int}$.

1. Implement the Jack-knife method for error estimation.

2. For the Ising model, look at ϵ_h as a function of the number of Jack-knife bins M (starting with $M = N$ and then decreasing it). Determine the largest value of M for which ϵ_h becomes independent of M and compare the value of N/M with the corresponding integrated autocorrelation time you determined in exercise 1.

[1] V. Ambegaokar, M. Troyer, Am. J. Phys., Vol. 78, No. 2, 150-157 (2010)