Exercise 04: Error analysis of a Markov Chain

Computational Physics WS20/21

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1 Introduction

In this week's exercise we want to find a proper estimate for the statistical error of a quantity estimated by generating a Markov Chain. The autocorrelation of elements in a Markov Chain, its effect on the error estimate and how one can reduce it by "blocking" (or "binning") and the bootstrap procedure are going to be discussed.

We want to simulate the Long Range Ising Model from last week's exercise 03 with the parameters $\beta J = 0.1$, $\beta h = 0.5$ and $n = 5$ (number of spin sites) for two different numbers of MD steps $N_{\mathrm{md}} = 4$ and $N_{\mathrm{md}} = 100$. We generate a long Monte Carlo Chain ($N = 12800$)

$$\{\phi\} = \{\phi_1, \phi_2, ..., \phi_N\} \tag{1}$$

and calculate the magnetization per spin

$$\{m\} = \{m_1 = m(\phi_1), m_2 = m(\phi_2), ..., m_N = m(\phi_N)\} \tag{2}$$

for each set of parameters.

1: *Plotting the history of the MC chain $\{m\}$ (generated in* `markov.py`*) in Fig. (1.1) shows, that for $N_{\mathrm{md}} = 4$, the metropolis hastings step results in a reject more often (it is $\phi_{k+1} = \phi$ more often) than for $N_{\mathrm{md}} = 100$. This is because the deviation between the Hamiltonian $H(p\prime, \phi\prime)$ with the new parameters $(p\prime, \phi\prime)$ and $H(p, \phi)$ scales with $\epsilon^2 = (1/N_{\mathrm{md}})^2$, which is obviously bigger for $N_{\mathrm{md}} = 4$.*

2 Autocorrelation

The $m_k = m(\phi_k)$ generated in the Markov Chain are obviously not random independet variables - they correlate. This correlation we want to analyze by calculating the

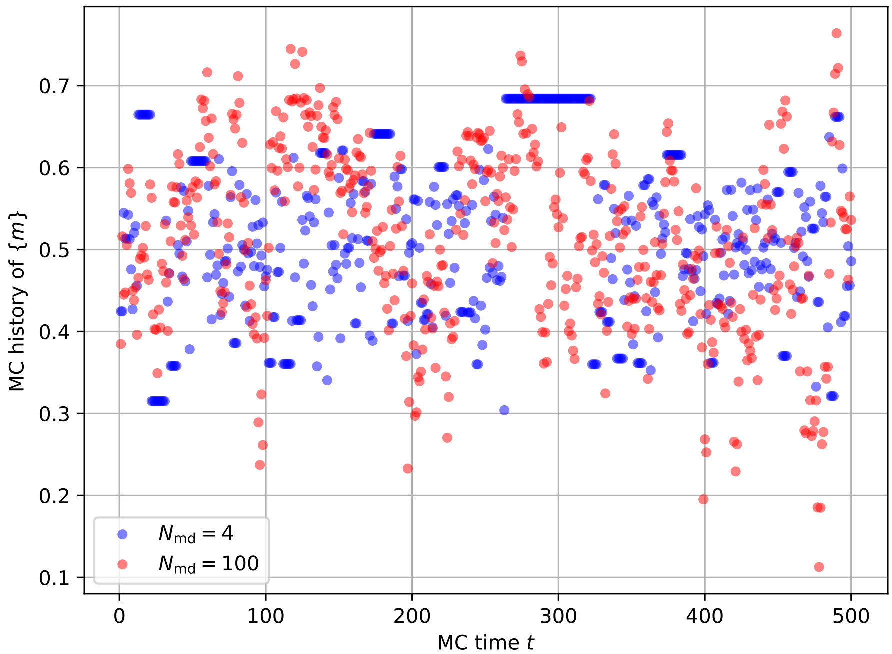

Figure 1.1: First 500 trajectories of the MC history of $\{m\}$ for both sets of parameters with $N_{\mathrm{md}} = 4$ and $N_{\mathrm{md}} = 100$.

autocorrelation function

$$\Gamma^{(m)}(|k-l|) = \langle (m(\phi_k) - \langle m \rangle)(m(\phi_l) - \langle m \rangle) \rangle \,. \tag{3}$$

In terms of $\tau = |k-l|$ the normalized autocorrelation function for a MC of length N with mean value $\bar{m}_N$ can be implemented as

$$\bar{\Gamma}^{(m)}(\tau) = \frac{1}{N-\tau} \sum_{k=1}^{N-\tau} (m_k - \bar{m}_N)(m_{k+\tau} - \bar{m}_N). \tag{4}$$

2: *The estimate for the autocorrelation $C(\tau) = \bar{\Gamma}^{(m)}(\tau)/\bar{\Gamma}^{(m)}(0)$ for both data sets ($N_{\mathrm{md}} = 4$ and $N_{\mathrm{md}} = 100$) is shown in Fig. (2.1). One can see, that for larger N_{md} the autocorrelation approaches zero faster for increasing τ.*

3 Blocking

From now on we use the data set with $N_{\mathrm{md}} = 100$ and proof how one can reduce the effects of autocorrelation by blocking the data. This means, reducing the length of the Markov Chain by creating a new list with averages of successive blocks of b elements of the original list (preserving its order). This list has now N/b elements.

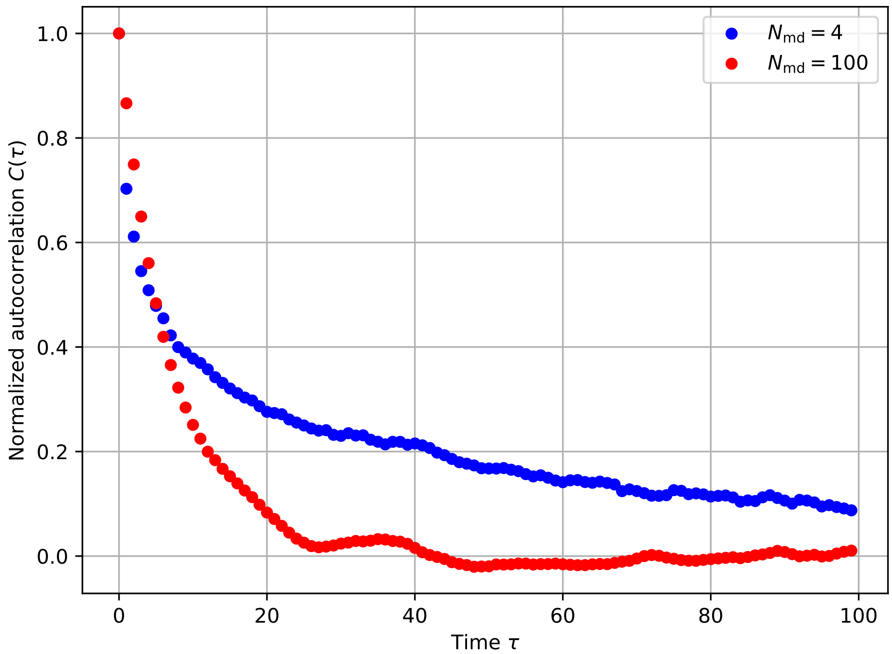

Figure 2.1: Estimate of autocorrelation $C(\tau) = \bar{\Gamma}^{(m)}(\tau)/\bar{\Gamma}^{(m)}(0)$ for both MCs with $N_{\mathrm{md}} = 4$ and $N_{\mathrm{md}} = 100$.

3: *The autocorrelation for different sets of blocked data for $b = 2, 4, 8, 16, 32$ and 64 is shown in Fig. (3.1). One can see, that for larger block sizes the autocorrelation approaches zero faster for increasing τ and is even negative at some τ for $b = 8$ and higher. However the flutuations increase for higher block sizes.*

The naive standard error $\sigma/\sqrt{N/b}$ for the blocked lists, with σ being their standard deviation, is plotted in Fig. (3.2). One can see, that it approaches a constant value $\sigma/\sqrt{N/b} \approx 0.0035$ for increasing block size b.

4 The bootstrap

Now we want to implement the bootstrap procedure (in `markov.py`) in order to get an unbiased estimate of the error. The bootstrap error can be calculated as follows:

- Given a list with N elements $\{m\}$, we generate a new list by randomply pulling N elements from $\{m\}$ (with replacement!).
- This we do N_{bs} times, creating a list of bootstrap lists.
- Now we calculate the mean of each bootstrap list, which gives a list of N_{bs} elements.

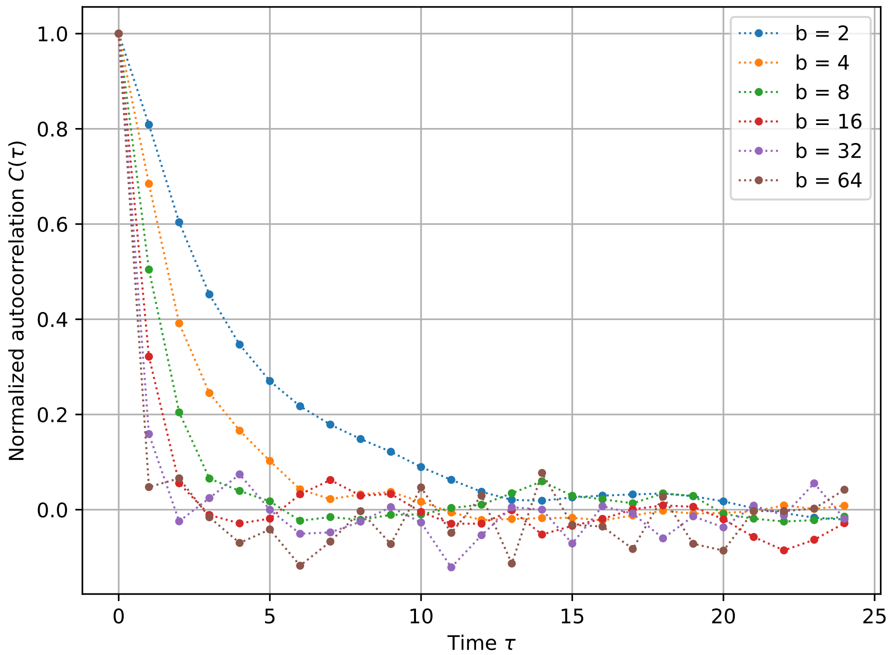

Figure 3.1: Estimate of autocorrelation $C(\tau)$ for blocked data sets with $b = 2, 4, 8, 16, 32$ and 64 ($N_{\mathrm{md}} = 100$).

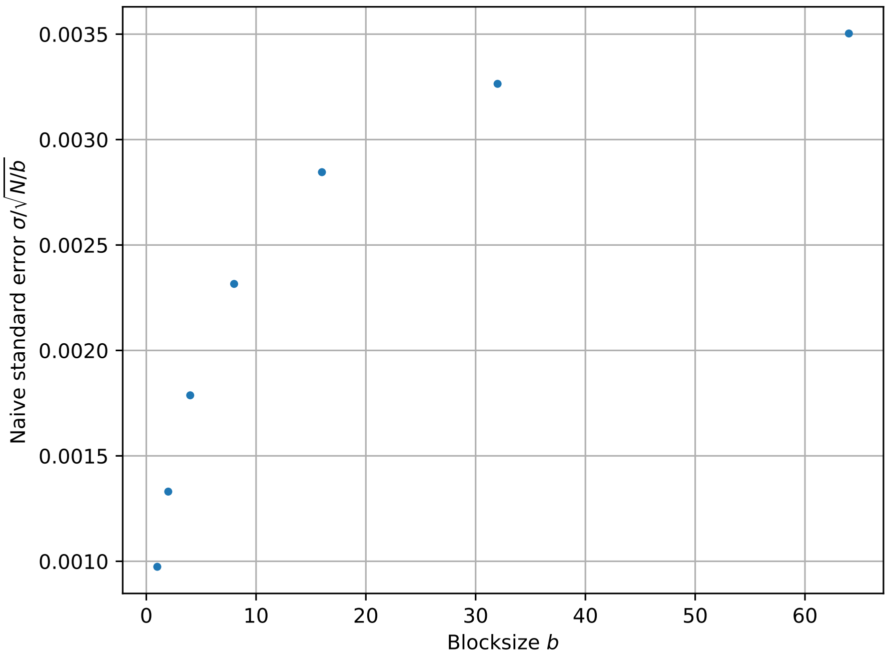

Figure 3.2: Naive standard error $\sigma/\sqrt{N/b}$ for the blocked data sets with $b = 2, 4, 8, 16, 32$ and 64 ($N_{\mathrm{md}} = 100$).

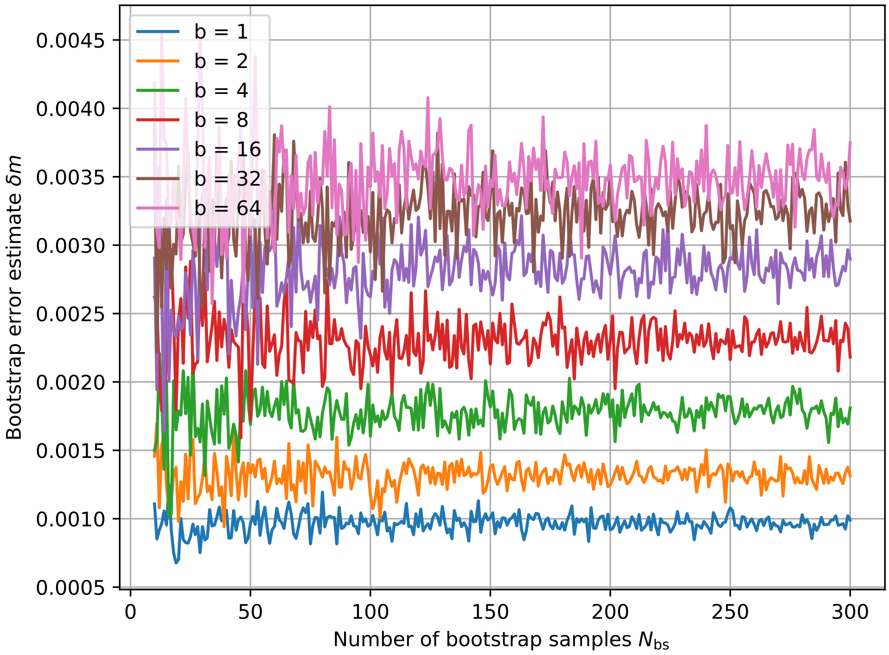

Figure 4.1: Dependece of the bootstrap error δm on the number of bootstrap lists $N_{\rm bs}$ for the blocked lists with $b = 2, 4, 8, 16, 32$ and 64.

- The bootstrap error δm is then the standard deviation of said list.

4: *The dependece of the bootstrap error on the number of bootstrap lists is shown in Fig. (4.1). The stability of the error increases greatly with* $N_{\rm bs}$*, meaning the the fluctuations around some mean value decrease. This mean value is roughly the same as the naive standard error calculated for the blocked lists, when comparing to Fig. (3.2).*

In order to verify how the differently calculated errors behave when taking more measurements (when increasing the length of the Markov Chain N), we plotted the bootstrap and the naive error against N. The result in Fig. (4.2) shows nicely how both errors decrease for increasing N.

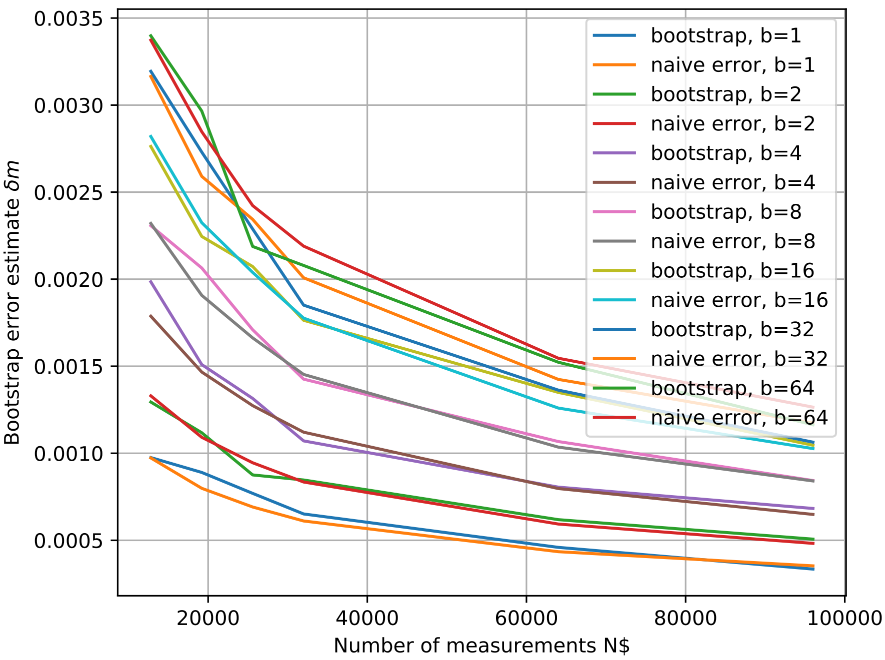

Figure 4.2: Dependece of the bootstrap and the naive error on the length of the Markov Chain N.