Computational Physics
Exercise 4

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1 Intro

In this exercise we study the long range Ising model. Its Hamiltonian is:

$$\mathcal{H}(s) = -\frac{1}{2}\frac{J}{N}\sum_{i,j} s_i s_j - h\sum_i s_i \tag{1}$$

The the second sum is over all spin sites and the first over all possible pairs of spin sites. This means that every spin interacts with every other spin. The factor of $\frac{1}{2}$ accounts for the double counting. We use a Hubbard-Stratonovich transformation to transform our problem from a discrete space into a continuous space. Then we can implement a HMC algorithm to vary the whole ensemble at once, instead of just single spins, when producing the desired distribution via a Markov chain. The detailed derivation can be found on exercise sheet 3.

We use the (corrected) implementation of this algorithm from exercise sheet 3.

In the following exercises we study the autocorrelation of the resulting markov chain and estimate the error of our estimate for the average magnetization.

2 Task 1

We call the data set with $N_{md} = 100$ HMC$_a$ and the data set with $N_{md} = 4$ HMC$_b$.

HMC$_a$ uses a higher number of integration steps than HMC$_b$. Therefore its integration is more precise and its trajectory changes less rapidly. The plateaus in HMC$_a$'s trajectory are the result of a chain of rejected steps, which are more likely for extreme values of phi and larger errors in the leapfrog step. Due to this HMC$_b$'s trajectory covers a smaller range of phi values than HMC$_a$'s.

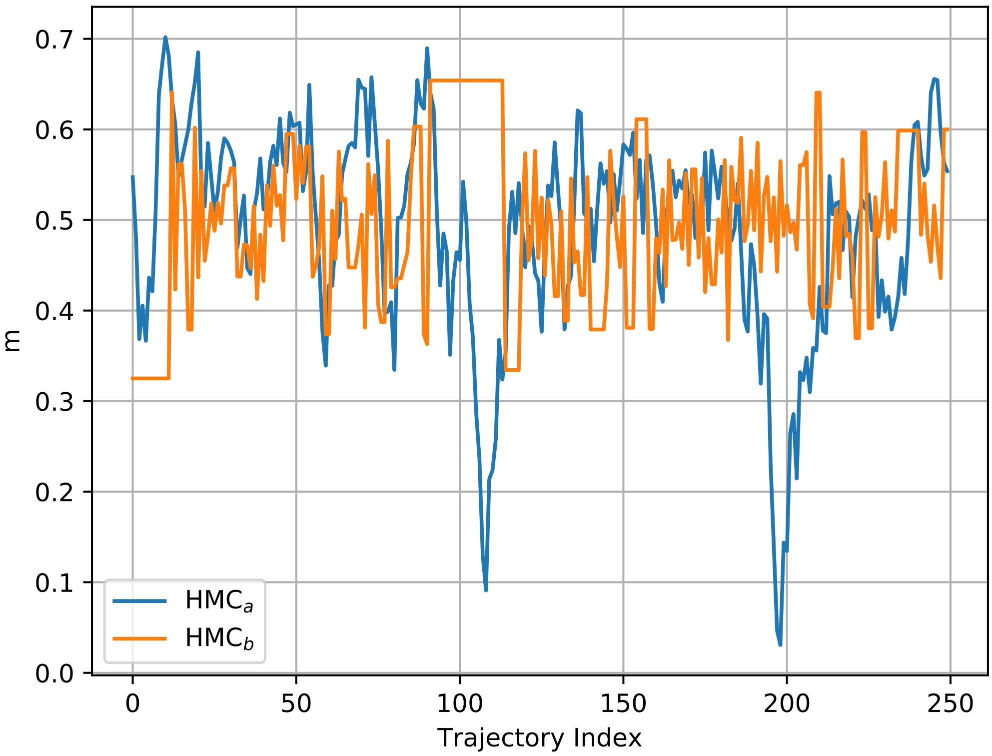

Figure 1: First 250 trajectories of HMC$_a$ and HMC$_b$ after thermalization

3 Task 2

The normalized autocorrelation function for HMC$_b$ falls faster in the beginning, but approaches 0 more slowly than for HMC$_a$.

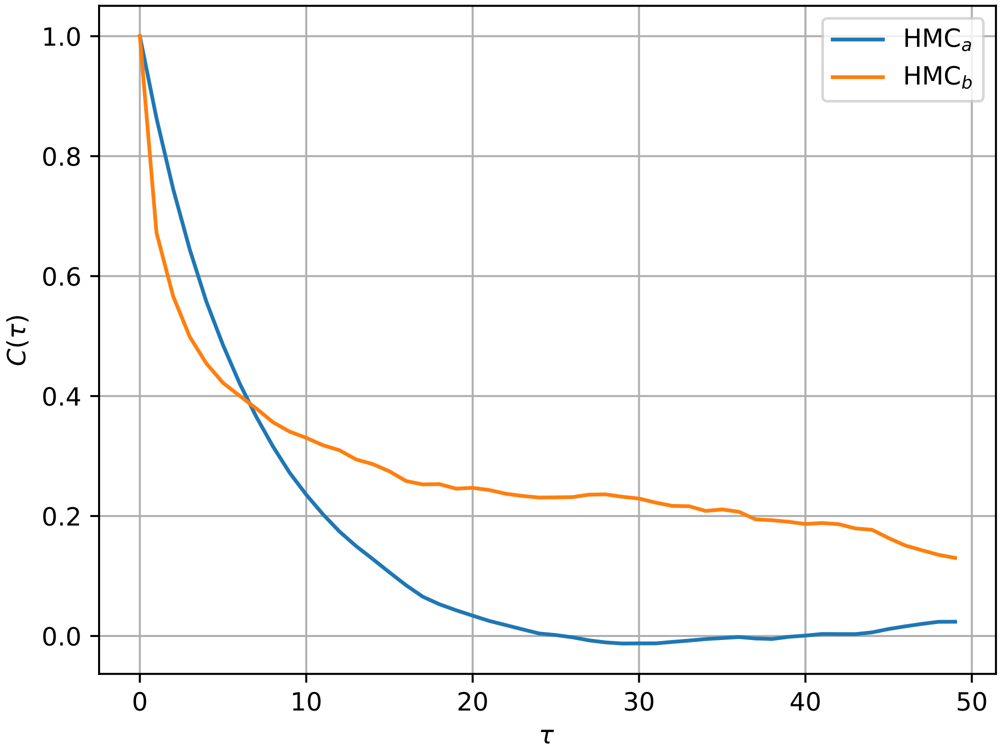

Figure 2: Normalized autocorrelation function for HMC$_a$ and HMC$_b$

4 Task 3

The autocorrelation decreases with increasing block size as expected. But our estimate for the (normalized) autocorrelation function $C(\tau)$ also becomes worse for large block sizes, because the sample of block, with which it is computed, becomes smaller.

The naive standard error seems to asymptotically approach a limit for large block sizes.

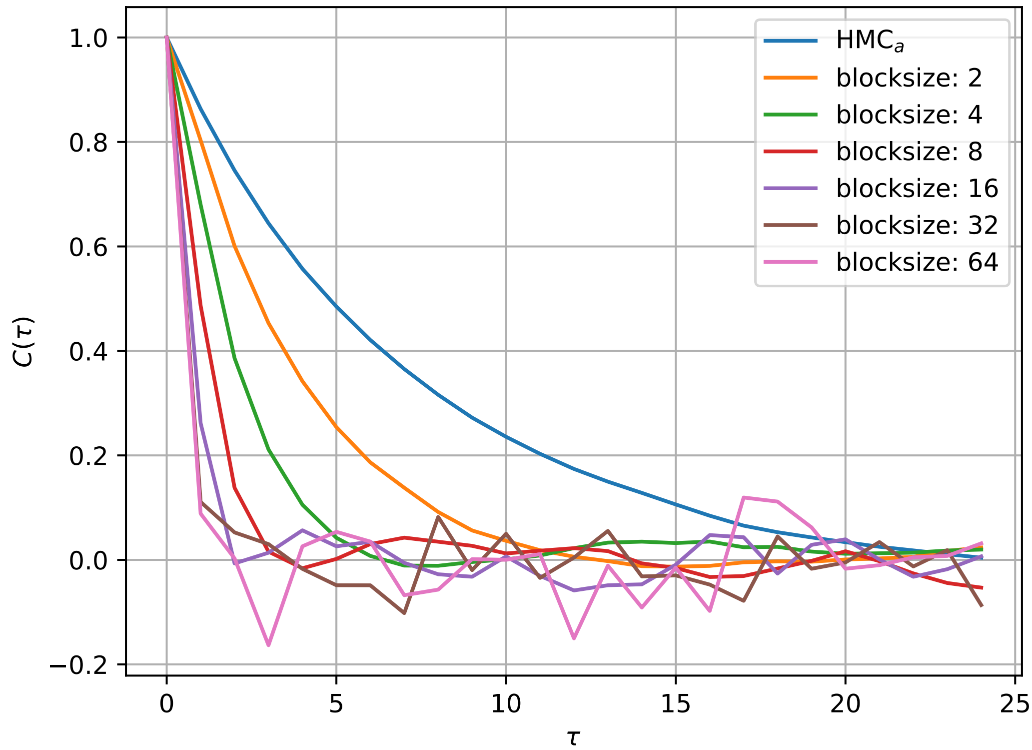

Figure 3: Normalized autocorrelation function for HMC$_a$ at various block sizes

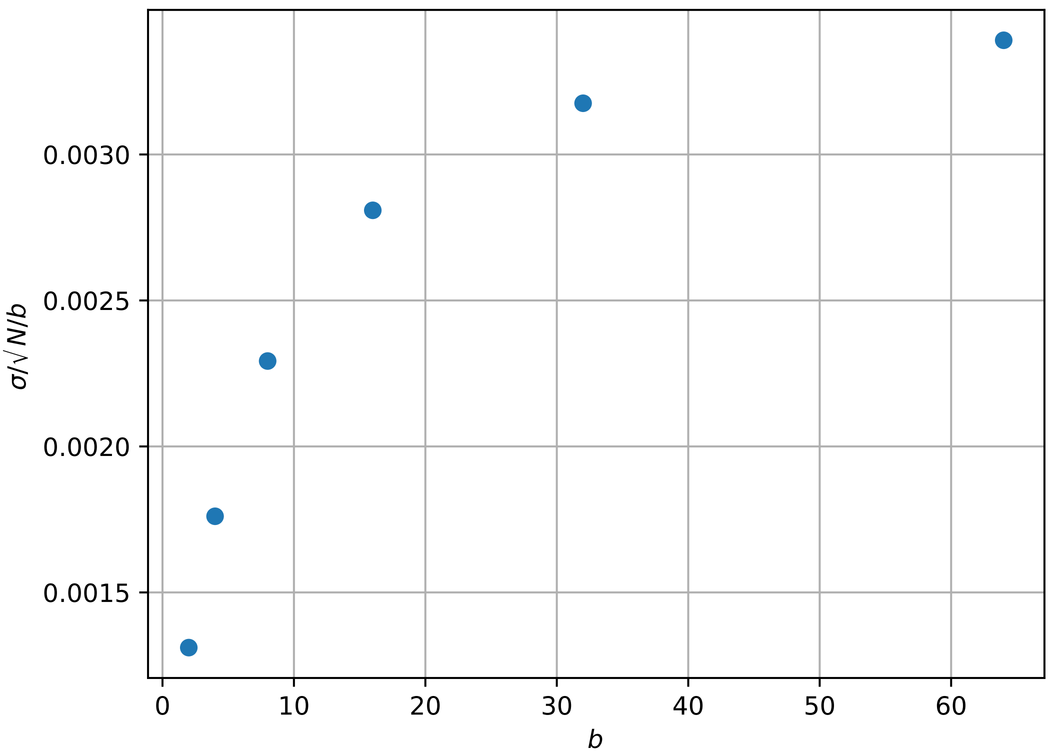

Figure 4: Naive standard error of the blocked lists

5 Task 4

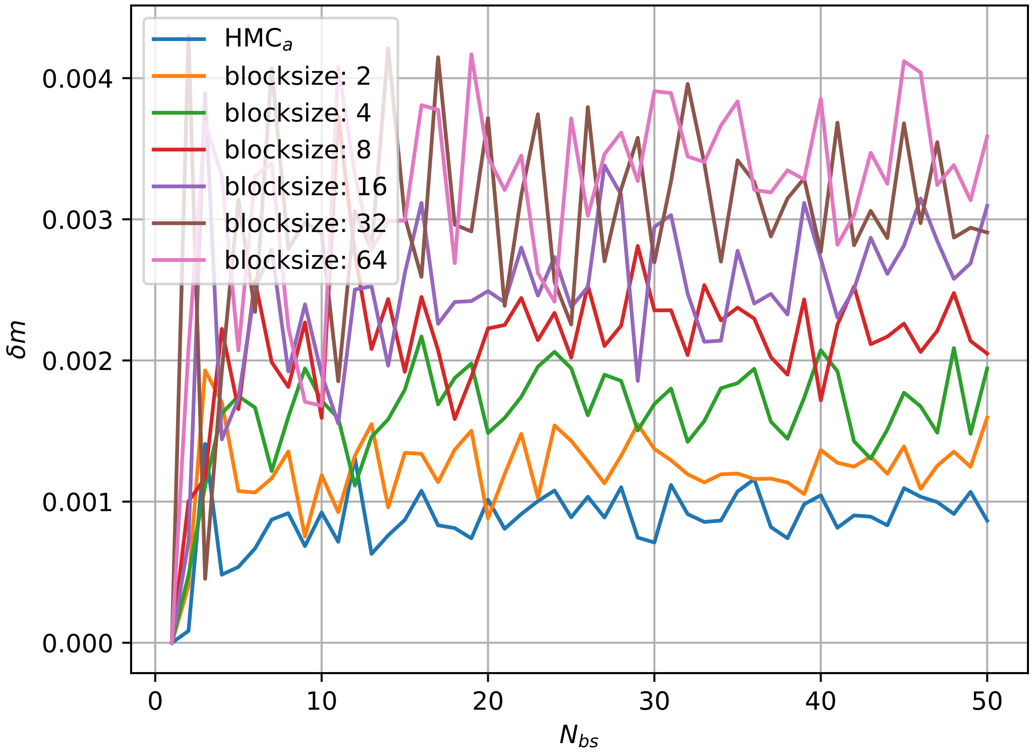

Figure 5: Bootstrap error δm in dependence of N_{bs}

The bootstrap error rises with block size and becomes less stable, probably because blocking reduces the sample size.

Naive error and bootstrap error are rather similar.

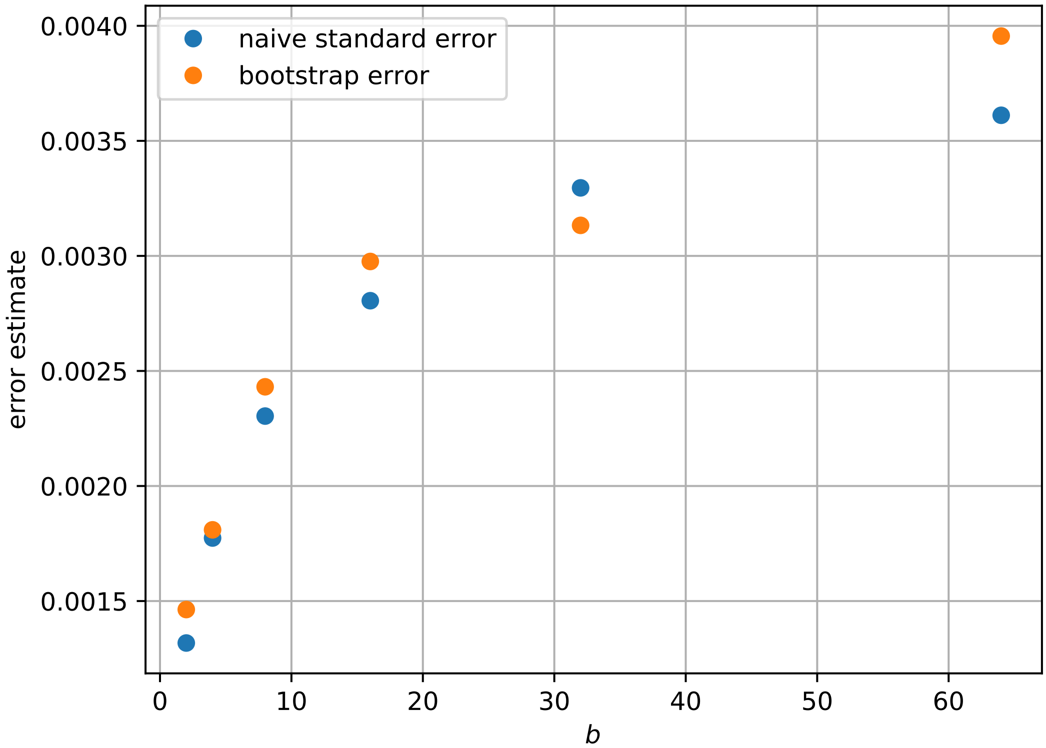

Figure 6: Comparison of the bootstrap error δm at $N_{bs} = 20$ with the naive standard error for varying block sizes b