Laboratory of Computational Physics

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1 Ising Model

In this section we study the statistical properties of a $2d$ Ising Model. We consider a system of 32×32 spins situated on the points of a regular square lattice with periodic boundary conditions in both directions. Each spin interacts with its nearest neighbours inside the lattice, with an Hamiltonian:

$$H = \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{1}$$

where the sum is taken only over the set of unordered pairs $\langle i, j \rangle$ such that σ_i and σ_j are nearest neighbours.

In order to obtain expectation values for physical quantities of the system we should be able to sum over the space of all the spin configurations, or at least to sample configurations from this space with probability:

$$P(\{\sigma\}) \sim \mathrm{e}^{-\beta H(\{\sigma\})} \tag{2}$$

which reproduces the integration measure of the functional integral. The obvious choice for numerical simulations is the second one, which we implement through Monte Carlo algorithms. In particular we focus on the Metropolis-Hastings (MH) and the Swendsen-Wang (SW) algorithms.

1.1 Thermalization

Since we do not know where to start in our Markov process, we first initialize the system in a random configuration (hot start) and then evolve for a certain Markov time until thermalization is reached. We expect the MH algorithm to be slower to thermalize because of the local update it employes as opposed to the cluster update of the SW algorithm.

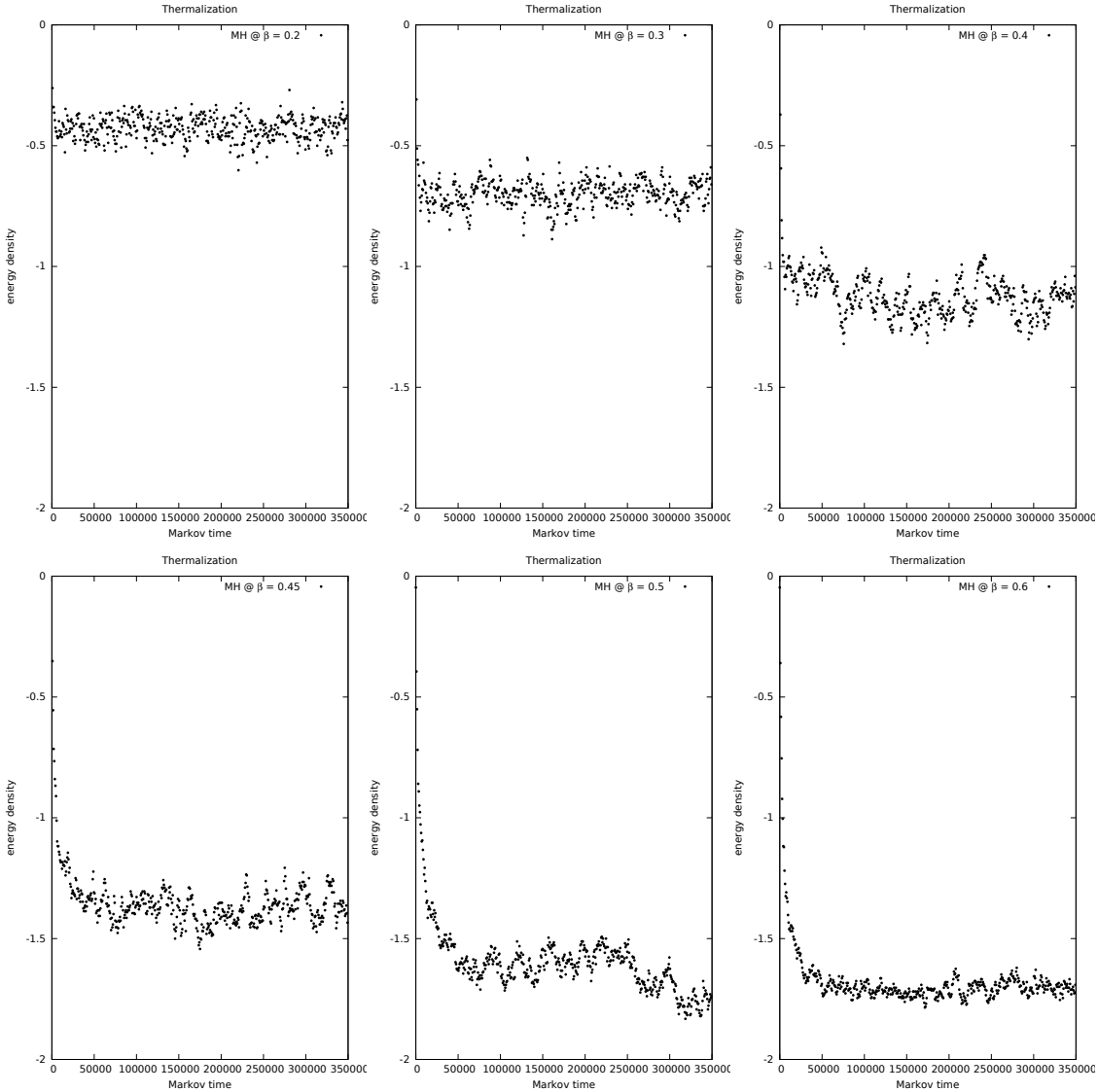

Figure 1. Plot of the energy density for the MH markov process at different values of β. The first $3.5 \cdot 10^6$ steps are drawn to show the thermalization process of the system.

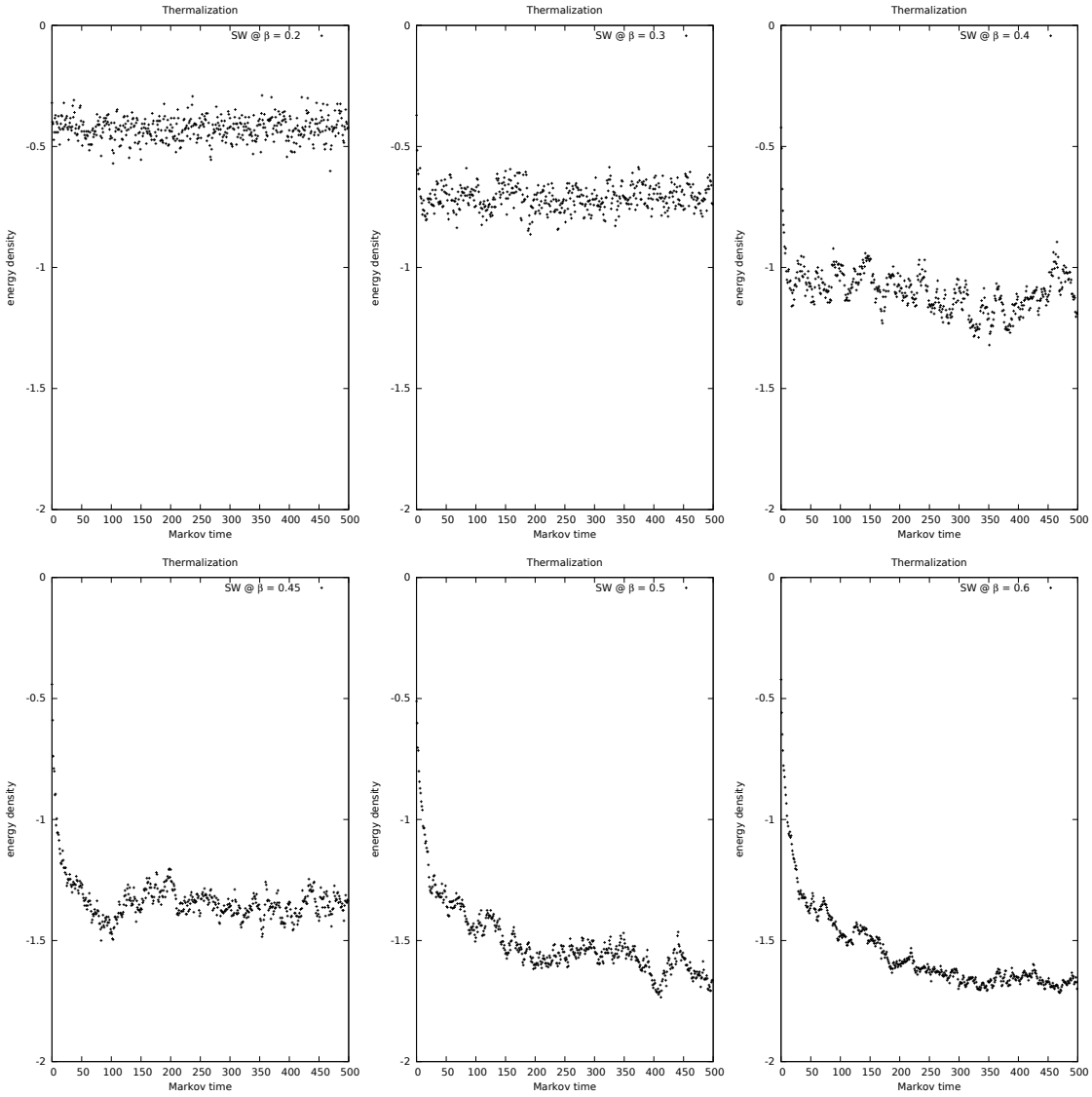

Figure 2. Plot of the energy density for the SW markov process at different values of β. This time we only present the first 500 steps.

As we can see from (Fig.1) the MH algorithm reaches thermalization after a Markov time two orders of magnitude larger than the lattice size 32×32 while the SW algorithm (Fig.2) takes only $\sim$500 steps. The reason for this discrepancy is that the MH update algorithm is local and therefore successive steps in the chain are strogly correlated, as we will see in section (1.2).

This effect is called *critical slowing down* and it tells us that when using local update algorithms only approximately every $N \times N$ sweeps through the lattice, a statistically independent measurement can be taken.

We also remark that for smaller values of β, the system energy can have larger fluctuations around its average and therfore thermal equilibrium is reached faster. For the rest of the simulations we used a thermalization time of $5 \cdot 10^6$ for MH and $5 \cdot 10^2$ for SW.

1.2 Autocorrelation

We now study the correlations present between consecutive configurations sampled by the two algorithms in order to obtain the characteristic time after which we can consider two configurations as statistically independent. This is called *integrated autocorrelation time* and is computed in the following way:

$$\tau_{\mathcal{O},\mathrm{int}} = \frac{1}{2} + \sum_{k=1}^{k_{\max}} R(k) \tag{3}$$

where $\mathcal{O}$ is the physical observable for which we compute autocorrelation and $R(k)$ is defined as:

$$R(k) = \frac{1}{(n-k)\,\sigma^2} \sum_{t=1}^{n-k} (\mathcal{O}_t - \mu)(\mathcal{O}_{t+k} - \mu) \tag{4}$$

here n is the total number of samples of $\mathcal{O}_t$ and μ, σ^2 are the mean and variance of the process. For a gaussian distributed process:

$$R(k) = \mathrm{e}^{-k/\tau_{\exp}} \tag{5}$$

We immediately see from (Fig.3) that the MH process is strongly correlated in time even for small values of the temperature:

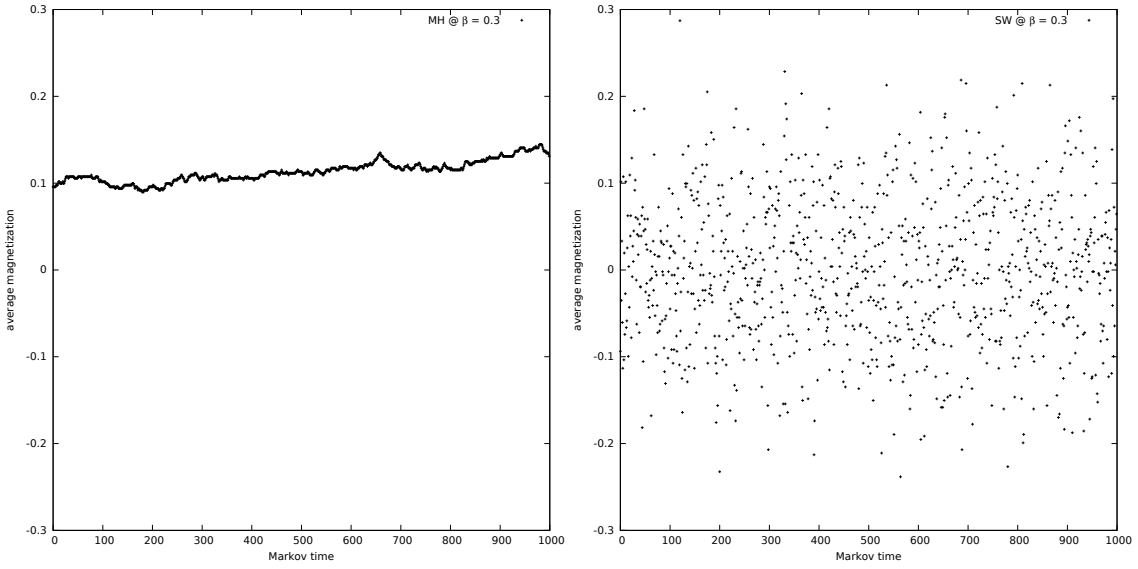

Figure 3. Comparison of the magnetization for the two algorithms at $\beta = 0.3$. (Left) MH (Right) SW.

Only on a larger time scale, the MH process can be regarded as weakly correlated (Fig.4):

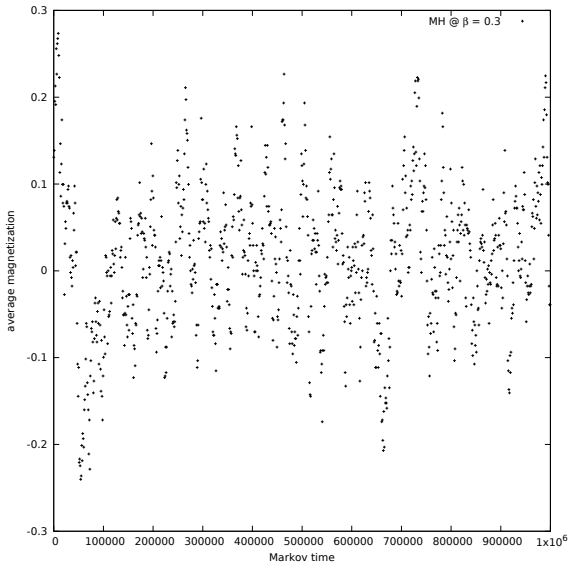

Figure 4. Average magnetization for the MH process observed on a larger time interval.

1.2.1 Autocorrelation time

We compute the autocorrelation time τ_e for the observable e (energy density).

1.3 Binning

In order to have a statistical ensamble of uncorrelated data we need to address the issue of autocorrelation in the Markov process. An easy and efficient way to do so is to split the data in non-overlapping blocks of the same size and then average over each block to obtain (almost)uncorrelated data for the observable $\mathcal{O}$ of interest. The blocks are also called *bins* and this method is called binning.

Consider an ensamble of $N = N_B \cdot k$ samples divided in N_B blocks of size k. For each block n we take the average of the observables $\mathcal{O}_i$ it contains and then obtain a block-observable $\mathcal{O}_{B,n}$:

$$\mathcal{O}_{B,n} = \frac{1}{k} \sum_{i=0}^{k-1} \mathcal{O}_{nk+i} \qquad n = 0, \dots, N_B - 1 \tag{6}$$

From a simple calculation we obtain that the error estimate on the mean value is:

$$\epsilon^2_{\bar{\mathcal{O}}} \equiv \sigma^2_{\bar{\mathcal{O}}} = \frac{\sigma^2_B}{N_B} = 2\,\tau_{\mathcal{O},\mathrm{int}}\,\frac{\sigma^2_{\mathcal{O}_i}}{N} \tag{7}$$

hence:

$$2\,\tau_{\mathcal{O},\mathrm{int}} = k\,\sigma^2_B / \sigma^2_{\mathcal{O}_i} \tag{8}$$

We study the dependence of the variance σ^2_B on the block size k. The observable we consider is the energy density e.

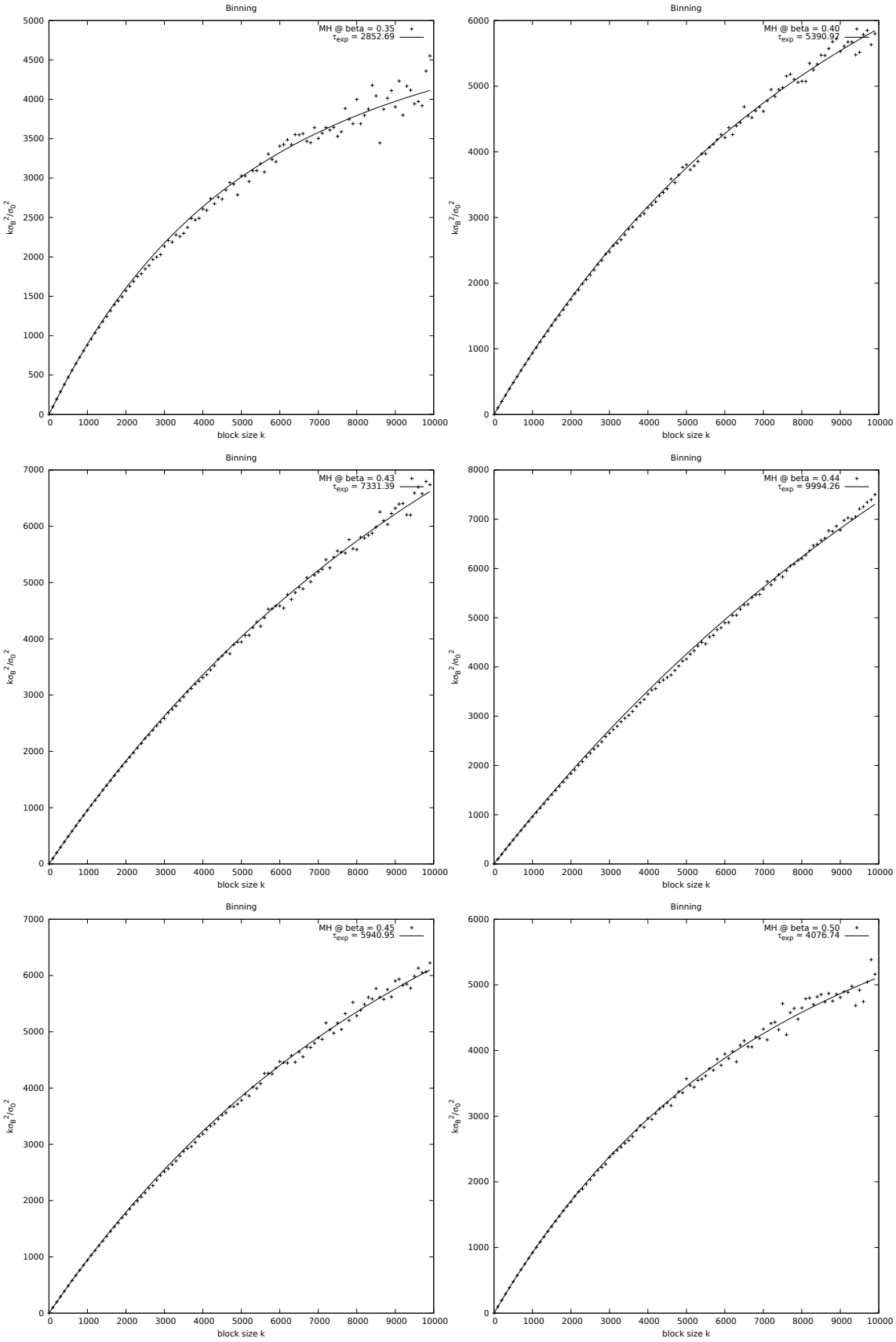

Figure 5. Binning analysis for the MH algorithm at various values of β.

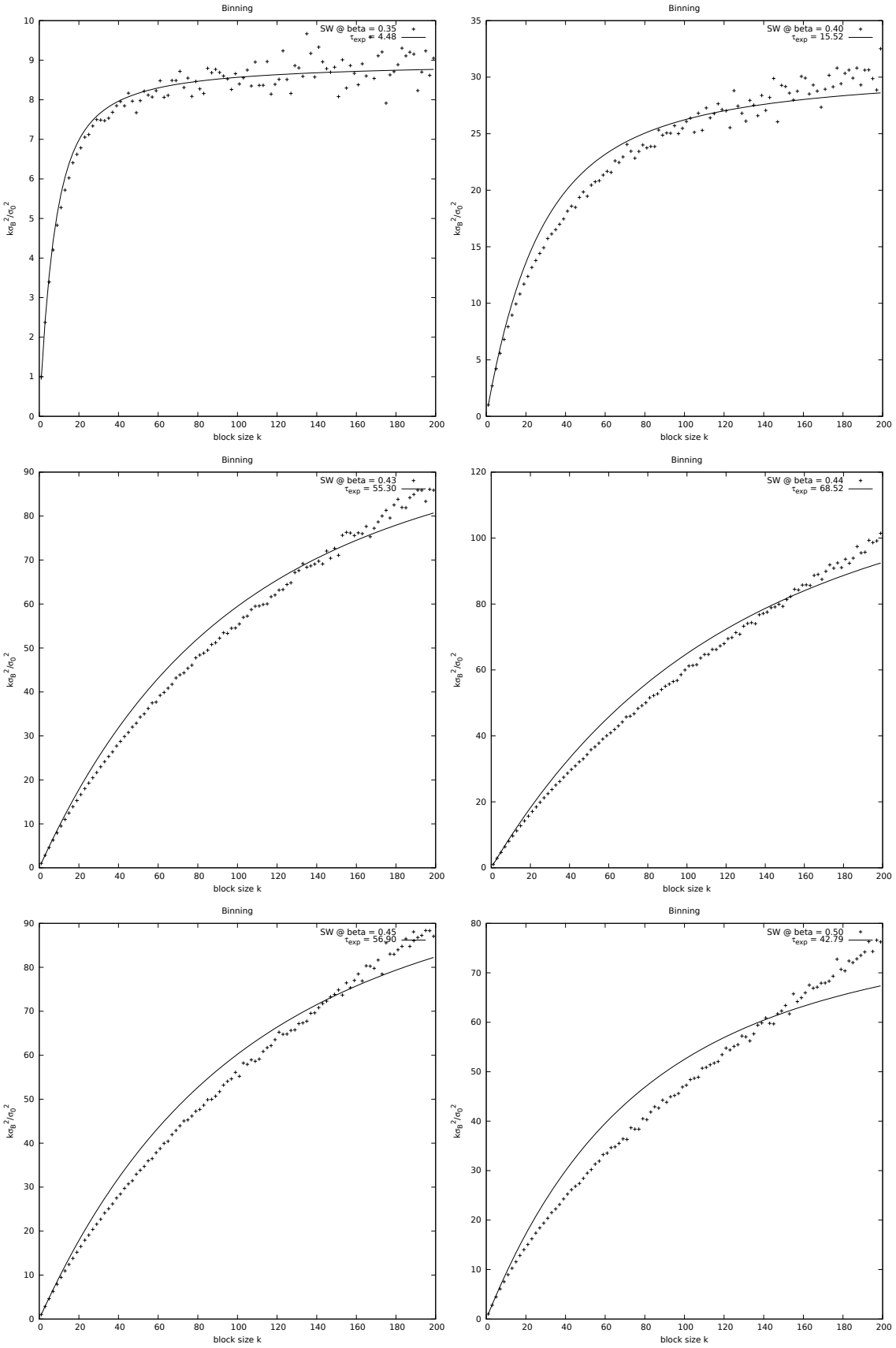

Figure 6. Binning analysis for the SW algorithm at various values of β.

Where we fitted the data using the formula:

$$k\,\sigma_B^2 \approx 2\,\tau_{\rm exp}\left(1-\frac{\tau_{\rm exp}}{k}\left(1-{\rm e}^{-\frac{k}{\tau_{\rm exp}}}\right)\right) \tag{9}$$

and we employed the self-consistent cut-off $k_{\rm max} < 6\,\tau_{\rm int}$.

The lowest value of k for which we can consider the data to be uncorrelated is obtained by looking at the point for which the signal for $k\,\sigma_B^2\,/\,\sigma_{\mathcal{O}_i}^2$ stabilizes and its first derivarive tends to zero. We call this point $\hat{k}(\beta)$. Since $\tau_{\rm exp}$ has a local maximum at the critical point, we take $\hat{k}(\beta_c)$ as the block size for the following simulations.

The value of $\hat{k}(\beta_c)$ for MH is taken to be $2\cdot 10^5$, almost two hundreds times the size of the lattice, while for SW it suffices to take $\hat{k}(\beta_c)\sim 400$.