Computational Physics

Exercise 5 - Multigrid simulation of the Gaussian model

Achilleas Patsias, Thomas Block

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The Gaussian model in one dimension has a Hamiltionian

$$H_a(u) = \frac{1}{a}\sum_{i=1}^{N}(u_i - u_{i-1})^2 \tag{1}$$

where a is the spacing between grid points, $N = L/a$ is the number of grid points and u is a real-valued field. For the simulation we use *Dirichlet boundary condition*

$$u(0) = u_0 = 0 \qquad u(L) = u_N = 0 \tag{2}$$

We can use Fourier decomposition of the field u

$$u_i = \sum_{k=1}^{N-1} c_k \sin\left(\frac{kl\pi a}{L}\right) \tag{3}$$

1 Analytic formulas

To check if the algorithms are working it is useful to know the analytic solutions to the expectation values of the magnetisation, the square of the magnetisation and the Hamiltonian, so we can compare them to the simulated results. The expectation value of an observable is given by

$$< O >= \frac{1}{Z}\prod_{i=1}^{N-1}\int_{-\infty}^{+\infty} du_i\; O\; \exp\left(-\beta H_a(u)\right) \tag{4}$$

with partition function Z

$$Z = \prod_{i=1}^{N-1}\int_{-\infty}^{+\infty} du_i\; \exp\left(-\beta H_a(u)\right) \tag{5}$$

The partition function Z is $N-1$ times a Gaussian integral

$$I = \int_{-\infty}^{+\infty} du_i\; \exp\left(-\frac{\beta}{a}(u_i - u_{i-1})^2\right) = \left(\frac{\pi a}{\beta}\right)^{\frac{1}{2}} \tag{6}$$

such that the partition function Z can be expressed as

$$Z = \left(\frac{\pi a}{\beta}\right)^{\frac{N-1}{2}} \tag{7}$$

The expectation value of the magnetisation $m = a/L\sum_{i=1}^{N-1} u_i$ is zero, because u_i is antisymmetric around 0, while the Gaussian exponential is symmetric around zero. The integral for positive u_i therefore cancels the integral for negative u_i, because both contributions have the same absolute value, but different signs.

The expectation value of the magnetisation squared is non-zero. With the Fourier decomposition we can write

$$m^2 = \left(\frac{a}{L}\right)^2 \left(\sum_{i=1}^{N-1} u_i\right)\left(\sum_{j=1}^{N-1} u_j\right) = \sum_{i=1}^{N-1}\sum_{j=1}^{N-1}\sum_{k=1}^{N-1}\sum_{l=1}^{N-1} c_k\, c_l\, \sin\left(\frac{ki\pi a}{L}\right)\, \sin\left(\frac{lj\pi a}{L}\right) \tag{8}$$

With the hint 4 on the sheet, we can see, that there are only non-zero contributions, when the indices are $k = l$ and $i = j$ such that we can write

$$m^2 = \left(\frac{a}{L}\right)^2 \left(\sum_{i=1}^{N-1} u_i\right)\left(\sum_{j=1}^{N-1} u_j\right) = \left(\frac{a}{L}\right)^2 \left(\sum_{i=1}^{N-1} u_i^2\right) \tag{9}$$

Both integrands in the expectation value are now symmetric and therefore the integral is non-zero:

$$< m^2 >= \frac{1}{Z} \prod_{i=1}^{N-1} \int_{-\infty}^{+\infty} du_i \left(\frac{a}{L}\right)^2 \left(\sum_{i=1}^{N-1} u_i^2\right) \exp\left(-\beta H_a(u)\right) \tag{10}$$

The integral splits up in $N-1$ sums of the form

$$I = \left(\frac{a}{L}\right)^2 \prod_{i=1}^{N-1} \int_{-\infty}^{+\infty} du_i\, u_i^2\, \exp\left(-\beta H_a(u)\right) = \tag{11}$$

$$\left(\frac{a}{L}\right)^2 \int_{-\infty}^{+\infty} du_i\, u_i^2\, \exp\left(-\frac{\beta}{a}(u_i - u_{i-1})^2\right) \times \prod_{i\neq 1}^{N-1} \int_{-\infty}^{+\infty} du_i\, \exp\left(-\beta H_a(u)\right) = \tag{12}$$

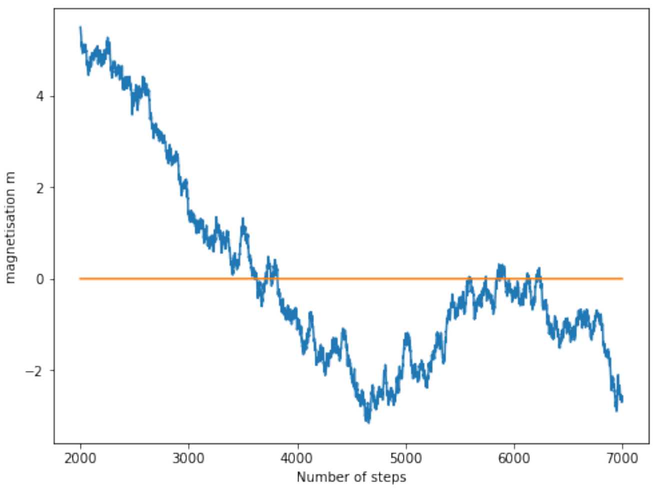
$$\left(\frac{a}{L}\right)^2 \left(\frac{\sqrt{\pi}}{2}\right)\left(\frac{a}{\beta}\right)^{\frac{3}{2}} \left(\frac{\pi a}{\beta}\right)^{\frac{N-2}{2}} = \left(\frac{a}{L}\right)^2 \left(\frac{a}{2\beta}\right)\left(\frac{\pi a}{\beta}\right)^{\frac{N-1}{2}} = \left(\frac{a^3}{2\beta L^2}\right) Z \tag{13}$$

This result is added $N-1$ times and devided by the partition sum Z and we finally get for the epectation value

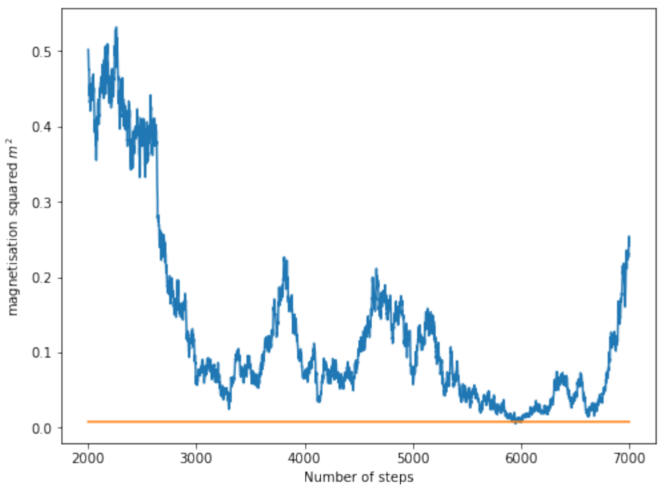
$$< m^2 >= (N-1)\left(\frac{a}{2\beta N^2}\right) \tag{14}$$

2 Implementation Metropolis-Hastings sweep

The code for this task can be found on the github page.



(a)



(b)

Figure 1: Magnetisation (left) and Magnetisation squared (right) for the Metropolis Hasting algorithm

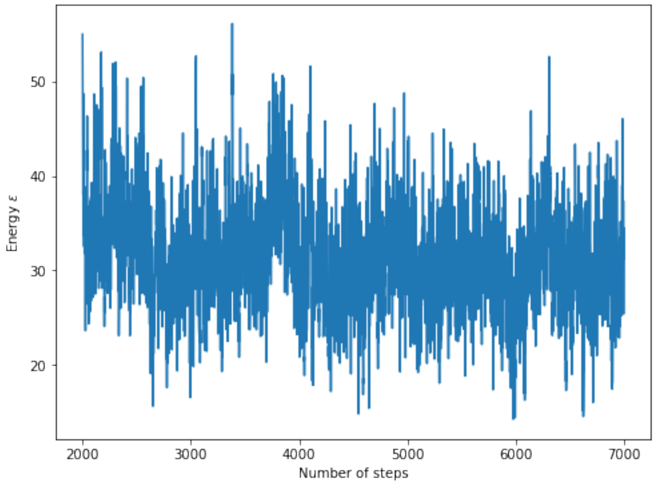


Figure 2: Energy for the Metropolis Hasting

Our theory was that the Metropolis-Hasting algorithm alone, does not work properly for this kind of situation and that is the reason that we should implement the Multigrid algorithm. Also we were not able to calculate the exact solution for the energy, although we used the Hamiltonian given in the sheet to calculate the energy explicitly.

3 $\Phi^{(2a)}$

This formula was given and so no points are needed.

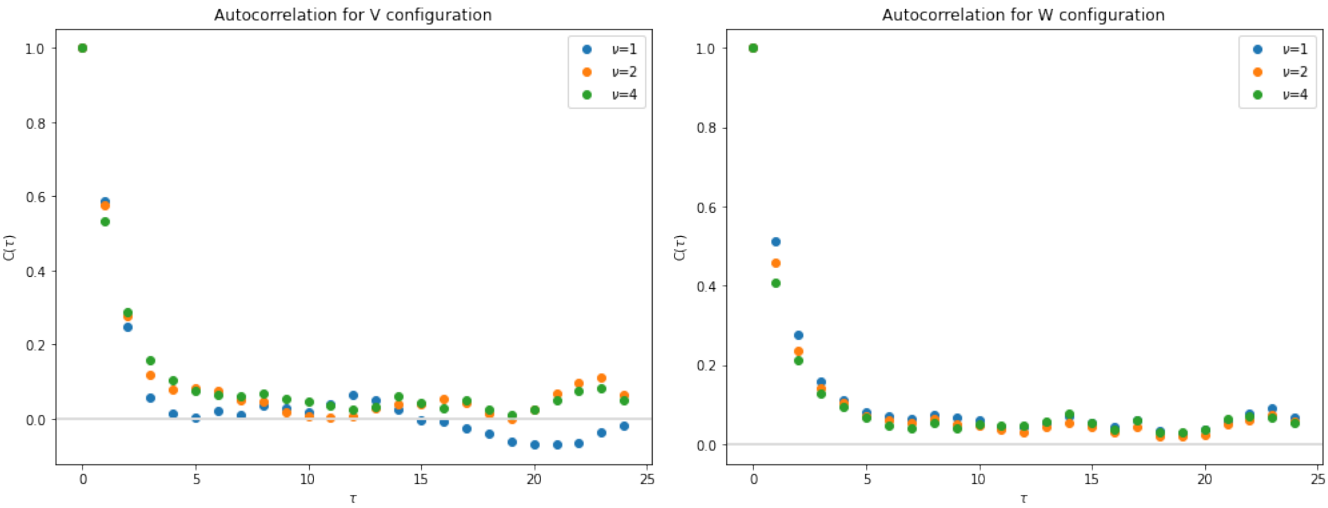
$$\phi^{(2a)} = \frac{1}{2a^2}[-s_{2k-2} + 2s_{2k} - s_{2k+2}] + \frac{1}{4}[\phi^{(a)}_{2k-1} + \phi^{(a)}_{2k} + \phi^{(a)}_{2k+1}]$$

with $s = \tilde{u}^{(a)}$.
The implementation of the recursion and prolongation functions can be found on github under the name FtC and CtF respectively

4 Implementation multigrid algorithm

The implementation of the Multi Grid algorithm can be found on github with the name *MG_simulation*

5 Test of implementation



(a) (b)

Figure 3: Autocorrelation of m^2 for the V configuration(left) and W configuration(right)