Exercises for Computational Physics (physics760)
WS 2020 / 21

Thomas Luu, Andreas Nogga, Marcus Petschlies, Andreas Wirzba

Exercise 5 (20 pts. total)

Homework (due Dec. 9 at 18:00)

Please note the due date of this homework. Submission of homework *requires* submitting your solutions (e.g. answers to questions, graphs, results in tabular form) in the form of a brief report (please no 100 page submissions!) **AND** a copy of your code that you used to do the simulations. Please address all questions and requirements written below in *italics* and red font in your homework report.

4 Multigrid simulation of the Gaussian model

In this homework we want to apply the multigrid technique to the simulation of the Gaussian model in 1 dimension. The microscopic degree of freedom is the real-valued field u with Hamiltonian given by

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

This can be seen the discretization of the continuous Hamiltonian

$$H(u) = \int_0^L dx \, \left(\partial u(x)\right)^2 \ .$$

In equation (1) a denotes the spacing between neighboring grid points and $N = L/a$. We use the *Dirichlet boundary condition* for field u, i.e.

$$\begin{aligned} u(0) &= u_0 = 0 \\ u(L) &= u_N = 0 \end{aligned} \tag{2}$$

and for this exercise we take N to be a power of 2. The Hamiltonian for the discretization with spacing a carries the latter as subscript. The partition sum for the system is given by

$$Z\left(\beta, N, a\right) = \prod_{i=1}^{N-1} \int_{-\infty}^{+\infty} du_i \, \exp\left(-\beta H_a(u)\right) \ . \tag{3}$$

With the simulation of the model, we will again seek to estimate expectation values of magnetization (squared) and energy. Since this is a new model for us, it is best to have some analytic results to compare to. Using Fourier decomposition with $u_\ell = \sum_{k=1}^{N-1} c_k \sin(k\pi\,\ell a/L)$, one has e.g. for the Hamiltonian

$$H_a(u) = \frac{2N}{a} \sum_{k=1}^{N-1} c_k^2 \sin^2\left(\frac{k\pi}{2N}\right) . \tag{4}$$

1: 1pt. *Based on the above Fourier decomposition determine the analytic formula for the expectation value* [1] *of*

- *the magnetization, defined by*

$$m = a/L \sum_{i=1}^{N-1} u_i \,, \tag{5}$$

- *its square* m^2 *and*
- *the energy / the Hamiltonian* H_a

As the Markov-chain kernel we use a sweep à la Metropolis-Hastings accept/reject with the following algorithm:

1. choose a site x for update , $x \sim U(\{1, \dots, N-1\})$
2. propose new $u'(x) = u(x) + r\,\delta$, with $r \sim U([-1,\, 1])$ and δ a fixed scale parameter
3. Metropolis accept / reject step

repeated $N-1$ times. [2]

2: 5pt. *Implement the above version of the Metropolis-Hastings sweep. Test your algorithm by sampling with* $\delta = 2.$, $N = 64$, $\beta = 1$. *Perform a measurement of the magnetization and energy after each sweep. Compare to the analytic results for the expectation values.*

Now let's look at the simulation using a multigrid algorithm. The main idea is to generate an update for the field $\tilde{u}^{(a)}$ at fine spacing a by simulating with a coarser discretization $2a$ (= fine-to-coarse restriction). From that we obtain a shift and add it to $\tilde{u}^{(a)}$ via an interpolation (= coarse-to-fine prolongation).

Fine-to-coarse restriction is given by using every 2nd grid point

$$u_i^{(2a)} = u_{2i}^{(a)} \,, \quad i = 0, \dots, N/2 \tag{6}$$

[1] The following formulas may be helpful. For $1 \le k, l \le N-1$:

$$\text{(I)} \quad \sum_{i=1}^{N-1} \sin(ik\pi/N) = \begin{cases} 0 & k \text{ even} \\ \cot(k\pi/(2N)) & k \text{ odd} \end{cases} \qquad \text{(II)} \quad \sum_{i=1}^{N-1} \sin(ik\pi/N)\,\sin(il\pi/N) = \frac{N}{2}\,\delta_{k,l}$$

$$\text{(III)} \quad \int_{-\infty}^{+\infty} dc\, c\, \exp\left(-\frac{c^2}{2\sigma^2}\right) = 0 \qquad \text{(IV)} \quad \int_{-\infty}^{+\infty} dc\, c^2\, \exp\left(-\frac{c^2}{2\sigma^2}\right) = \sqrt{2\pi\sigma^2}\,\sigma^2 \,.$$

[2] $y \sim U(X)$ means random variable y is distributed according to uniform distribution on the set X.

Coarse-to-fine prolongation uses linear interpolation

$$I_{(2a)}^{(a)}\, u^{(2a)} = \begin{cases} u_{i/2}^{(2a)} & i = 0, 2, \ldots, N \\ \left(u_{(i-1)/2}^{(2a)} + u_{(i+1)/2}^{(2a)}\right)/2 & i = 1, 3, \ldots, N-1 \end{cases} \tag{7}$$

Consider now the generalized Hamiltonian

$$H_a(u) = \frac{1}{a} \sum_{i=1}^{N} (u_i - u_{i-1})^2 + a \sum_{i=1}^{N-1} \phi_i^{(a)}\, u_i\,. \tag{8}$$

with an external field $\phi^{(a)}$. The prolongation $u^{(a)} = \tilde{u}^{(a)} + I_{(2a)}^{(a)}\, u^{(2a)}$ leads to a decomposition

$$\begin{aligned} H_a\left(u^{(a)}\right) &= H_a\left(\tilde{u}^{(a)}\right) + H_{2a}\left(u^{(2a)}\right)\,, \\ H_{2a}\left(u^{(2a)}\right) &= \frac{1}{2a} \sum_{i=1}^{N/2} \left(u_i^{(2a)} - u_{i-1}^{(2a)}\right)^2 + 2a \sum_{i=1}^{N/2-1} \phi_i^{(2a)}\, u_i^{(2a)}\,. \end{aligned} \tag{9}$$

3: 4pt. *Give the explicit form of $\phi^{(2a)}$: how does the coarse-level external field $\phi^{(2a)}$ depend on the fine-level fields ? Implement the restriction and prolongation functions.*

Now we have all ingredients to compile the multigrid simulation algorithm, which reads:
At the current level with spacing a

1. do ν_{pre} pre-coarsening sweeps at the current level; if the current level is the coarsest level, proceed to step 5;
2. generate the next coarser level for grid spacing $2a$, i.e. determine $\phi^{(2a)}$ and thus the Hamiltonian H_{2a} (to use in sweeps on the coarser level)
3. *heads up: recursive step!* do γ multigrid cycles for the coarser level; start initially with $u^{(2a)} \equiv 0$;
4. update the current $u^{(a)}$ by

$$u^{(a)} \leftarrow u^{(a)} + I_{(2a)}^{(a)}\, u^{(2a)} \tag{10}$$

   with $u^{(2a)}$ as obtained in step 3;

5. do ν_{post} post-prolongation sweeps at the current level

This is a recursive definition: steps 1 to 5 apply as well to any level that is entered. On the finest level we start with zero external field. The number of sweeps ν_{pre} and ν_{post} should be adjustable for each level. For simplicity we set $a = 1$ for the finest level and $\beta = 1$ for the inverse temperature.

4: 7pt. *Implement the above multigrid algorithm for n_{level} levels and number of cycles γ.*

5: 3pt. *Test your implementation with $N = 64$, $\delta = 2$, $\gamma = 1, 2$ and $n_{\text{level}} = 3$. Moreover, set the following number of sweeps for coarsest to finest level: $\nu_{\text{pre}} = \nu_{\text{post}} = 4, 2, 1$.*
Plot the autocorrelation function of the squared magnetization as defined in eq. (5) for this choice of parameters.