Worksheet 6: Finite-Size Scaling and the Ising Model

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Contents

1 General Remarks

- Deadline for the report is **Tuesday, 5th February 2013, 10:00**.
- On this worksheet, you can achieve a maximum of 20 points.
- The report should be written as though it would be read by a fellow student who attends to the lecture, but does not do the tutorials.
- To hand in your report, send it to your tutor via email
  - Olaf (`olenz@icp.uni-stuttgart.de`; Thursday, 14:00 – 15:30)
  - Jens (`smiatek@icp.uni-stuttgart.de`; Friday, 8:00 – 9:30)
- Please attach the report to the email. For the report itself, please use the PDF format (we will *not* accept MS Word DOC files!). Include graphs and images into the report.

- If the task is to write a program, please attach the source code of the program, so that we can test it ourselves.
- The report should be 5–10 pages long. We recommend to use LaTeX. A good template for a report is available.
- The worksheets are to be solved in groups of two or three people.

On this worksheet, you will combine all the methods and skills that you have obtained during the term and use them to compute the critical temperature T_c and the critical exponents β_m and ν of the two-dimensional Ising model.

All files that are required for this tutorial can be found in the archive `templates.tar.gz` that can be downloaded from the lecture's homepage.

As on the previous worksheet, we will perform simulations of the two-dimensional Ising model on a $(L \times L)$ square lattice. $\sigma_{i,j} \in$ denotes the spin at lattice position (i, j).

The (total) energy of the system is defined by

$$E = \frac{1}{2} \sum_{i=0}^{L-1} \sum_{j=0}^{L-1} E_{i,j} \tag{1}$$

where

$$E_{i,j} = -\sigma_{i,j}(\sigma_{i-1,j} + \sigma_{i+1,j} + \sigma_{i,j-1} + \sigma_{i,j+1}) \tag{2}$$

The system uses periodic boundary conditions, *i.e.*

$$\begin{aligned} \sigma_{-1,j} &= \sigma_{L-1,j} & \qquad \sigma_{L,j} &= \sigma_{0,j} \\ \sigma_{i,-1} &= \sigma_{i,L-1} & \qquad \sigma_{i,L} &= \sigma_{i,0} \end{aligned}$$

As an observable, we are interested in the (mean) *energy per site* e, which is defined by

$$e = \langle \frac{E}{L^2} \rangle$$

and the (mean) *magnetization per site* m

$$m = \langle |\mu| \rangle \tag{3}$$

where

$$\mu = \frac{1}{L^2} \sum_{i=0}^{L-1} \sum_{j=0}^{L-1} \sigma_{i,j} \tag{4}$$

2 Speeding up the Simulation

The Ising Monte-Carlo simulation from the last worksheet is written in pure Python. Unfortunately, when the size of the lattice L grows, the performance of the simulation is too low.

Task (4 points)

- Speed up the simulation program by implementing all or parts of it in C/Cython.
- Give reasons why you rewrote what part of the program.

Hints

- To generate random numbers in C, use the random number generator from the *GNU Scientific Library* (GSL), as the default random number generator (RNG) has a too short period for MC simulations. The file `cising-impl.c` contains functions that demonstrate the usage of the GSL RNG.
- The files `cising.pyx`, `cising-impl.c`, `setup.py` and `test_cising.py` contain a small sample Python/Cython/C-program that generates a list of random numbers. From the program, you should be able to pick all parts that you need to do the task.

3 Determine Equilibrium Values and Errors

In this task, your job is to perform simulations of the two-dimensional Ising model for different lattice sizes L and measure the equilibrium values of the magnetization and the energy and their errors.

Task (4 points)

- Run simulations with $L \in \{16, 64\}$ for $T \in \{1.0, 1.1, 1.2, \ldots, 4.9, 5.0\}$
- Determine equilibrium values and errors of M and E for all of these plots
- Plot M and E (with errorbars) as a function of T for the different system sizes.
- Add the exact curve for $L = 4$ from the last worksheet.
- How do the curves depend on L?

Hints

- If you want to store simulation data to a file, remember the module `pickle`.
- To reduce the file size, you can use the module `gzip`. Open the file with `gzip.open`, then all following operations will work on a compressed file.

4 Finite Size Scaling

4.1 Determining T_c

Task (4 points)

- Implement the Binder parameter $U = 1 - \frac{1}{3}\frac{\langle \mu^4 \rangle}{\langle \mu^2 \rangle^2}$.
- Measure the Binder parameter for $L \in \{4, 16, 64\}$ and $T \in \{2.0, 2.02, 2.04 \ldots, 2.38, 2.4\}$.
- Plot U vs. T for the different values of L.
- Determine T_c to a precision of ± 0.02.

Hints Note that you need a pretty good accuracy of U to determine T_c.

4.2 Estimating β_m

Task (4 points)

- Perform simulations at T_c with different $L \in \{8, 16, 32, 64, 128\}$
- Plot M against L in double logarithmic scale.
- From the theory, what is the scaling law of the magnetization, *i.e.* how does the magnetization depend on L?
- Try to estimate β_m from the curve, given that $\nu = -1$ for a two-dimensional Ising system.

4.3 The Master Curve

When plotting $ML^{\beta_m/\nu}$ against $tL^{-\nu}$, for different values of L and $t = |1-T/T_c|$ (*reduced temperature*), all data should fall on a single master curve.

Task (4 points)

- Use all of your data from this worksheet and plot the master curve for the estimated value of β_m from the last task.
- Try to get a better estimate for β_m via the following procedure: make plots of mL^a against $tL^{-\nu}$ with different values of a and select one where all data points are on the same curve. Always plot the data with errorbars, so that one can visually check if they fit within the estimated error. Provide the best-looking plot and your estimated value of β_m.