

Computational Physics – Exercise 4: Monte Carlo methods

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Exercise:

1D and 2D Ising model

- 1D model: The energy of a configuration is given by

$$E = -\sum_{n=1}^{N-1} S_n S_{n+1}$$

- Use the MMC method to compute the average energy U / N and specific heat C / N per spin for $T = 0.2, 0.4, \dots, 4$ and $N = 10, 100, 1000$
 $N_{\text{samples}} = 1000, 10000$
 - Free boundary conditions

Exercise:

1D and 2D Ising model

- 1D model: To check the results, compare with the exact analytical solution.

$$\begin{aligned} Z &= \sum_{\{S_1, \dots, S_N\}} \exp\left(\beta \sum_{n=1}^{N-1} S_n S_{n+1}\right) = \sum_{\{S_1, \dots, S_N\}} \prod_{n=1}^{N-1} e^{\beta S_n S_{n+1}} \\ &= \sum_{\{S_1, \dots, S_N\}} e^{\beta S_1 S_2} \prod_{n=2}^{N-1} e^{\beta S_n S_{n+1}} = 2 \cosh \beta \sum_{\{S_2, \dots, S_N\}} \prod_{n=2}^{N-1} e^{\beta S_n S_{n+1}} \\ &= 2(2 \cosh \beta)^{N-1} \end{aligned}$$

$$U / N = -\frac{N-1}{N} \tanh \beta \quad , \quad C / N = -\frac{\beta^2}{N} \frac{\partial U}{\partial \beta} = \frac{N-1}{N} (\beta / \cosh \beta)^2$$

Example output

1D Ising model, $N = 1000$

T	beta	U_MC	C_MC	U_theory	C_theory	acc
0.400E+01	0.250E+00	-0.245E+00	0.586E-01	-0.245E+00	0.588E-01	0.83
0.380E+01	0.263E+00	-0.257E+00	0.651E-01	-0.257E+00	0.647E-01	0.82
0.360E+01	0.278E+00	-0.271E+00	0.717E-01	-0.271E+00	0.715E-01	0.80
0.340E+01	0.294E+00	-0.286E+00	0.804E-01	-0.286E+00	0.794E-01	0.79
0.320E+01	0.313E+00	-0.303E+00	0.852E-01	-0.303E+00	0.887E-01	0.77
0.300E+01	0.333E+00	-0.322E+00	0.981E-01	-0.322E+00	0.996E-01	0.75
0.280E+01	0.357E+00	-0.342E+00	0.115E+00	-0.343E+00	0.113E+00	0.72
0.260E+01	0.385E+00	-0.366E+00	0.131E+00	-0.367E+00	0.128E+00	0.70
0.240E+01	0.417E+00	-0.393E+00	0.146E+00	-0.394E+00	0.147E+00	0.67
0.220E+01	0.455E+00	-0.426E+00	0.170E+00	-0.426E+00	0.169E+00	0.63
0.200E+01	0.500E+00	-0.462E+00	0.195E+00	-0.462E+00	0.197E+00	0.59
0.180E+01	0.556E+00	-0.504E+00	0.229E+00	-0.505E+00	0.230E+00	0.54
0.160E+01	0.625E+00	-0.554E+00	0.269E+00	-0.555E+00	0.270E+00	0.49
0.140E+01	0.714E+00	-0.613E+00	0.317E+00	-0.613E+00	0.318E+00	0.43
0.120E+01	0.833E+00	-0.681E+00	0.383E+00	-0.682E+00	0.371E+00	0.35
0.100E+01	0.100E+01	-0.761E+00	0.403E+00	-0.762E+00	0.420E+00	0.26
0.800E+00	0.125E+01	-0.847E+00	0.429E+00	-0.848E+00	0.438E+00	0.17
0.600E+00	0.167E+01	-0.932E+00	0.370E+00	-0.931E+00	0.370E+00	0.07
0.400E+00	0.250E+01	-0.987E+00	0.125E+00	-0.987E+00	0.166E+00	0.01
0.200E+00	0.500E+01	-0.993E+00	0.193E+00	-0.100E+01	0.454E-02	0.01



Exercise:

1D and 2D Ising model

- 2D model: The energy of a configuration is given by

$$E = -\sum_{i=1}^{N-1} \sum_{j=1}^N S_{i,j} S_{i+1,j} - \sum_{i=1}^N \sum_{j=1}^{N-1} S_{i,j} S_{i,j+1}$$

- Use the MMC method to compute the average energy U / N^2 and specific heat C / N^2 per spin for $T = 0.2, 0.4, \dots, 4$ and $N = 10, 50, 100$ (free boundary conditions)
- Also compute the average magnetization per spin

$$M = \frac{\sum_{\{S_{1,1}, \dots, S_{N,N}\}} \sum_{i,j=1}^N S_{i,j} e^{-\beta E}}{\sum_{\{S_{1,1}, \dots, S_{N,N}\}} e^{-\beta E}}$$

and compare with the exact result for the infinite system

$$M / N^2 = \begin{cases} \left(1 - \sinh^{-4} 2\beta\right)^{1/8} & \text{if } T < T_c = \frac{2}{\ln(1 + \sqrt{2})} \\ 0 & \text{if } T > T_c \end{cases}$$

Exercise:

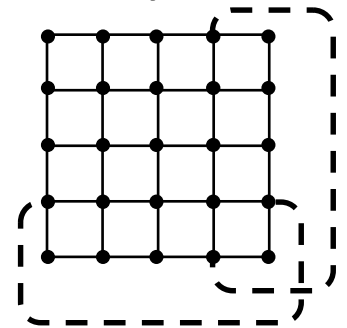
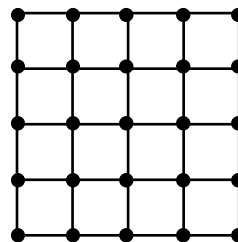
1D and 2D Ising model

- 2D model: make 3 plots of the results of the average energy U / N^2 , specific heat C / N^2 and magnetization M / N^2 per spin and put the data for $N = 10, 50, 100$ on the same plot
 - $N_{\text{samples}} = 1000, 10000$
- Interpret the results in terms of a phase transition from a state with magnetization zero to a state with definite magnetization

Exercise:

1D and 2D Ising model

- Boundary conditions: Simulations are performed on finite systems → How to treat edges (boundaries) of the lattice?
 - Periodic boundary conditions: wrap the d -dimensional lattice on a $(d+1)$ -dimensional torus
 - Effectively eliminates boundary effects, but the system is still characterized by the finite lattice size
 - Free boundary conditions



Report

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- Filename: **Report_4_Surname1_Surname2.pdf**, where Surname1 < Surname2 (alphabetical order).
Example: Report_4_Jin_Willsch.pdf (Do not use “umlauts” or any other special characters in the names)
- Content of the report:
 - Names + matricule numbers + e-mail addresses + title
 - **Introduction**: describe briefly the problem you are modeling and simulating (write in complete sentences)
 - **Simulation model and method**: describe briefly the model and simulation method (write in complete sentences)
 - **Simulation results**: show figures (use grids, with figure captions !) depicting the simulation results. Give a brief description of the results (write in complete sentences)
 - **Discussion**: summarize your findings
 - **Appendix**: Include the listing of the program

Due date: 10 AM, May 19, 2022