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 $T = 0.2, 0.4, \ldots, 4$ 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.

$$Z=\sum_{\{S_1,\ldots,S_N\}}\exp(\beta\sum_{n=1}^{N-1}S_nS_{n+1})=\sum_{\{S_1,\ldots,S_N\}}\prod_{n=1}^{N-1}e^{\beta S_nS_{n+1}}$$

$$=\sum_{\{S_1,\ldots,S_N\}}e^{\beta S_1S_2}\prod_{n=2}^{N-1}e^{\beta S_nS_{n+1}}=2\cosh\beta\sum_{\{S_2,\ldots,S_N\}}\prod_{n=2}^{N-1}e^{\beta S_nS_{n+1}}$$

$$=2\left(2\cosh\beta\right)^{N-1}$$

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

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 $T = 0.2, 0.4, \ldots, 4$ and $N = 10, 50, 100$ (free boundary conditions)
- Also compute the average magnetization per spin

$$M = \sum_{\{S_{1,1},\ldots,S_{N,N}\}} \sum_{i,j=1}^{N} S_{i,j} e^{-\beta E} \Big/ \sum_{\{S_{1,1},\ldots,S_{N,N}\}} e^{-\beta E}$$

and compare with the exact result for the infinite system

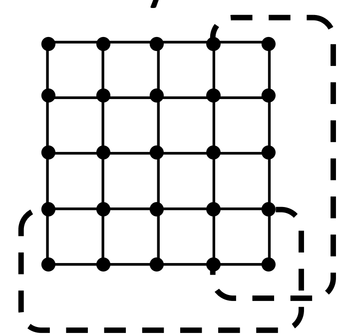
$$M/N^2 = \begin{cases} \left(1 - \sinh^{-4} 2\beta\right)^{1/8} & \text{if} \quad T < T_\mathrm{C} = \dfrac{2}{\ln(1+\sqrt{2})} \\ 0 & \text{if} \quad T > T_\mathrm{C} \end{cases}$$

Exercise:
1D and 2D Ising model

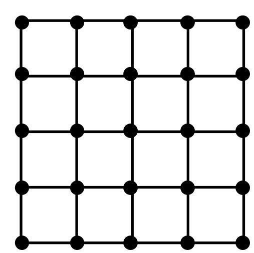
- 2D model: make 3 plots of the results of the average energy U/N^2, specific heat C/N^2 and magnetization M/N^2 per spin and put the data for $N = 10, 50, 100$ on the same plot
  - $N_{\text{samples}} = 1000, 10000$
- Interpret the results in terms of a phase transition from a state with magnetization 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: Follow the instructions given by the tutors
- Content of the report:
  - Names + matricle 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 14, 2024