Computational Physics – Exercise 6: 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 $N = 10, 100, 1000$

$$N_{samples} = 1000, 10000$$

  - Free boundary conditions

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Exercise:
1D and 2D Ising model

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

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

$$= \sum_{\{S_1,..,S_N\}} e^{\beta S_1 S_2} \prod_{n=2}^{N-1} e^{\beta S_n S_{n+1}} = 2\cosh\beta \sum_{\{S_2,..,S_N\}} \prod_{n=2}^{N-1} e^{\beta S_n S_{n+1}}$$

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

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

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

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

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
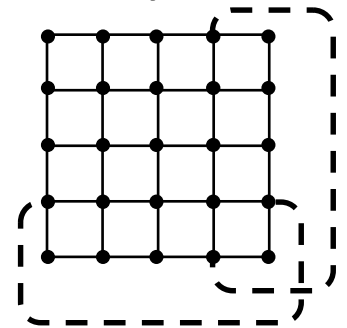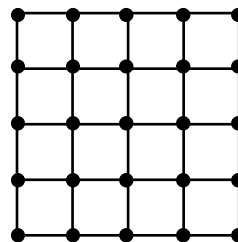
Report

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- Filename: Report_6_Surname1_Surname2.pdf, where Surname1 < Surname02 (alphabetical order). Example: Report_6_Jin_Lagemann.pdf (Do not use "umlauts" or any other special characters in the names)

- 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: 5 PM, June 16, 2020