Report 1

Report 1: MCMC simulation of square lattice Ising model

General information

- Please solve both 1-1 and 1-2.
  - (optional) means it is not mandatory. So, even if you do not solve the task, in principle, you can get the perfect score. When you include it, you may get additional points.
- Please include your name and student id in your report.
- Please submit it through **ITC-LMS.**
  - In case you cannot use ITC-LMS, please submit it by email.
    - I will send a reply when I receive your reports.
    - If you do not receive any response, please contact me.
- **Deadline: 2023 June 13th**

Report problem 1-1: Auto-correlation functions

- Discuss the auto-correlation function and its relaxation time as follows

  1. Perform MCMC simulation of the square lattice Ising model.
     - Please try at least two algorithms: Metropolis and Swendsen-Wang (cluster)
     - If you prefer, you may simulate another model, such as MCMC simulation of cubic lattice Ising model, MD simulation of LJ particle, …
       - In those cases, please do not forget to mention the algorithms you used.
  2. Calculate (and plot) auto-correlation functions of magnetization (<M>) and squared magnetization (<M^2>).
     - When you select a different model, please choose your observables accordingly.
  3. **Discuss** behaviors of auto-correlation functions and correlation time by varying temperatures and system sizes (# of spins).
     - Please discuss in what cases the correlation time becomes longer.
       - Note that when the system size is too small, you may not observe explicit parameter dependences.
     - Please discuss the differences between <M> and <M^2> correlation times.
     - Please compare correlation times between Metropolis and Swendsen-Wang.

Report problem 1-1: Auto-correlation functions

4. Based on the previous discussion, consider how we should set MC steps (simulation time) to obtain reliable data when we change temperature and system size.
    - Remember the relationship between the correlation time and the statistical error.

Note:

To discuss the correlation time, it might be useful to use the integrated correlation time defined as

$$\tau = \int_0^\infty \frac{C(t)}{C(0)} dt \sim \sum_{t=0}^{T} \frac{C(t)}{C(0)}.$$

Report problem 1-1: Tips

- For MCMC simulation, you can use
  - Your own code
  - Open-source software
  - My sample codes (python) (Ising-auto.ipynb or .py in Report1.zip).
    - In order to run the sample codes, you need numpy, matplotlib, and numba modules in addition to the python3.
    - See also the header of the codes.
- In order to obtain correct auto-correlation function, we need to take care about the “thermalization" (initial state dependence) mentioned in the lecture.
  - In the case of the sample codes of Ising model,
    When you increase the system size
    or
    when you change the temperature,
    you may need to increase the "thermalization" parameter, which sets MC steps discarded before calculating auto-correlation functions.
  - It is also important to sample sufficiently long time, to evaluate the correlation time.

Report problem 1-2: Phase transition

- Investigate the phase transition of the $L \times L$ square lattice Ising model as follows.
  1. Perform MCMC for at least three system sizes, such as L=16, 32, and 64. If your computer environment allows, it is recommended to include larger than L=32 (e.g., L=48, 64, …).
     - Please explicitly write down the algorithm you used, e.g., Metropolis, Heatbath, Swendsen-Wang, ...
  2. Plot the figures of the squared magnetization and the specific heat as functions of temperature. (You can also include figures of other quantities.)
  3. Try to (roughly) estimate the transition temperature, T_c, from the behaviors of specific heat and the square magnetization.
     - Please note the expected behaviors in the thermodynamic limit (infinite L limit).
       - The specific heat diverges at T_c.
       - The magnetization is zero and finite when $T > T_c$ and $T < T_c$, respectively.

Report problem 1-2: Phase transition

4. Next, plot the "binder ratio of magnetization" and estimate the crossing temperature.
   - As explained in the lecture, this crossing temperature becomes an accurate estimate of T_c.
5. **Discuss** the above estimations of T_c.
   - Please compare them to the exact value of T_c. (You can find it in the lecture slide).
   - Please don't forget to mention the statistical errors.
6. (optional) Try the finite-size scaling of the binder ratio by using your estimate of T_c.
   - You may see a data collapse independent of L by adequately changing the horizontal axis. (As explained in the lecture, we need the critical exponent ν. Here you can use its exact value $\nu=1$, or you may estimate it from the data collapse.)
7. (optional) If you are interested, please compare TRG and MCMC.
   - Please note that MCMC contains statistical errors, while there are systematic errors in TRG.

Report problem 1-2: Tips

- For MCMC simulation, you can use
  - Your own code
  - Open source softwares
  - My sample codes (python) (Ising-obs.ipynb or .py in Report1.zip).
    - In order to run the sample codes, you need numpy, matplotlib, and numba modules in addition to python3.
    - See also the header of the codes.
- In order to obtain accurate results corresponding to the thermal equilibrium, MC steps are so important.
  - As I mentioned in the lecture, e.g., when the thermalization is too short compared with the correlation time, your result may be biased by the initial condition.
    - Note that even if the thermalization is sufficient, the statistical error also depends on the correlation time.
  - As you will experience in the report problem 1-1, the correlation time depends on the temperatures and the system sizes.

Report problem 1-2: Tips

- For TRG, you can use
  - Your own code
  - My sample codes (python) (Ising-trg.ipynb in Report1.zip).
    - In order to run the sample codes, you need numpy, matplotlib, and numba modules in addition to python3.
    - See also the header of the codes.
- To compare the results obtained by MCMC and TRG, Ising-comp.ipynb miggt be useful.

* It might be helpful to see

https://github.com/TsuyoshiOkubo/Introduction-to-Tensor-Network

There are lecture materials related to TRG.

(Unfortunately, they are presented in Japanese)

Important notice

- Please check that you can perform the report problem in your environment as soon as possible.
  - I recommend google colab to run my sample codes.
    - Please see a short instruction in the No.4 (or No.5) slide.
- If you have any troubles or questions, please ask me
  - by email: t-okubo@phys.s.u-tokyo.ac.jp
  - or come to my office **Sci. Bldg. #1 950.**
    (It is better to get an appointment by email.)
    If you have any troubles, please send us an email:
    t-okubo@phys.s.u-tokyo.ac.jp
- If a report contains only figures, you will lose lots of points.
  - Please include *explanations* and *discussions* about your results. These are essential!
- In case you use ChatGPT or other similar systems, please mention them in the report.