Computational Physics – Lecture 7: Monte Carlo methods II

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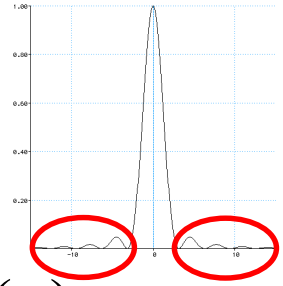
Contents

- Importance sampling Monte Carlo methods
  - Numerical integration
  - Metropolis Monte Carlo for the Ising model
    - Exercise

Importance sampling Monte Carlo:
Numerical integration



- Importance sampling:
  - Rewrite the integral $I = \int_a^b f(x)dx$ as $I = \int_a^b \frac{f(x)}{p(x)} p(x)dx$

    where $p(x)$ is a probability distribution function

    $\int_a^b p(x)dx = 1$
  - Choose $p(x)$ such that it is close to $f(x)$ but simpler
  - The integral is evaluated by generating random numbers according to $p(x)$

Importance sampling Monte Carlo:
Numerical integration

– Choosing N values of x with the probability $p(x)$ the estimate for the integral reads

$$I_N = \frac{1}{N}\sum_{n=1}^{N}\frac{f(x_n)}{p(x_n)}$$

- Because of the normalization of $p(x)$ all the numbers x_n are in $[a,b]$

– In general: $p(x)$ should be chosen to mimic the form of $f(x)$ as closely as possible in order to make $f(x)/p(x)$ slowly varying (small variance)

Importance sampling Monte Carlo: Ising model

- Ising model with N spins→ 2^N possible spin configurations (states)
  - →Ising model can often be difficult to analyze numerically (brute force)
  - →simulate the Ising Model using Monte Carlo methods
- Consider 1D Ising model with $h = 0$ to introduce the Metropolis Monte Carlo method:

$$H = -J \sum_{<n,m>} S_n S_m$$

Importance sampling Monte Carlo:
Ising model

- The energy of a particular arrangement $\{S_1,\ldots,S_N\}$ of N spins is defined as

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

- According to statistical mechanics, the probability to realize a configuration with energy E is given by ($k_B = 1$, choice of units)

$$P(\text{configuration}) = e^{-E/T} \Big/ \sum_{\{S_1,\ldots,S_N\}} e^{-E/T}$$

The average energy U and specific heat C at temperature $T = 1/\beta$ are given by

$$U = \frac{\sum_{\{S_1,\ldots,S_N\}} E e^{-\beta E}}{\sum_{\{S_1,\ldots,S_N\}} e^{-\beta E}}, \quad C = \beta^2 \left(\frac{\sum_{\{S_1,\ldots,S_N\}} E^2 e^{-\beta E}}{\sum_{\{S_1,\ldots,S_N\}} e^{-\beta E}} - U^2 \right)$$

Importance sampling Monte Carlo:
Metropolis Monte Carlo method

- Number of possible arrangements of N spins $\{S_1,...,S_N\}$ is 2^N ➔ the number of possible energies E is 2^N
- For $N > 100$ it would take a lot of computer time to sum all the terms ➔ Monte Carlo sampling over all possible $\{S_1,...,S_N\}$
- However, for each configuration of spins $\{S_1,...,S_N\}$, statistical mechanics gives us the expression for $P(\text{configuration})$ but in fact, we do not know the value $P(\text{configuration})$ unless we can sum over all possible configurations of spins to determine the numerator in $P(\text{configuration})$
  - A conundrum?
- Fundamental question: How can we generate random configurations of spins if we do not know the values of $P(\text{configuration})$?
- Very general solution: Metropolis Monte Carlo method (1953)
  - Very simple algorithm
  - Mathematical proof is much more complicated than its application

Importance sampling Monte Carlo: Metropolis Monte Carlo method

- The MMC algorithm
  1. Pick a configuration of spins $\{S_1,...,S_N\}$
  2. Calculate the energy $E = E(S_1,...,S_N)$ of this configuration
  3. Do loop, count is N, the number of spins
  4. Pick a spin, say $j = r * N + 1$, randomly
  5. Calculate the change of the energy E' if we would flip spin j, meaning that $S_j \leftarrow -S_j$
  6. Compute $q = P(\text{new conf.}) / P(\text{old conf.}) = P(E + E') / P(E) = e^{-\beta E'}$
     - Note that the unknown numerator does not enter!
  7. If $q > r$ accept the spin flip, i.e. do $S_j \leftarrow -S_j$ and $E \leftarrow E + E'$
     - Every time we write " r ", it is implied that we call the random number generator
  8. End of Do loop

Importance sampling Monte Carlo:
Metropolis Monte Carlo method

- The MMC algorithm is like a "black box" that generates random configurations $\{S_1,...,S_N\}$ which are distributed according to the unknown distribution $P(\text{configuration})$
- Sounds like magic? In a way it is.
- How does it work?
  - Importance sampling: it "searches" the space of configurations such that it finds the most important ones
  - Modest price to pay: This search can take (very) long
  - Proof that it works: Theory of Markov chains
- Very general algorithm: The "energy" E can be almost any function of any type of variables
  - Many different applications: Statistical mechanics, optimization, machine learning, …

Importance sampling Monte Carlo: Markov chain

- Define a stochastic (random) process at discrete times labeled consecutively $t_1, t_2, t_3, \ldots$, for a system with a finite set of possible states $Y_1, Y_2, Y_3, \ldots$, and denote by X_t the state the system is in at time t
- Consider the conditional probability

$$P\left(X_{t_n} = Y_{i_n} \mid X_{t_{n-1}} = Y_{i_{n-1}}, X_{t_{n-2}} = Y_{i_{n-2}}, \ldots, X_{t_1} = Y_{i_1}\right)$$

Importance sampling Monte Carlo: Markov chain

- A Markov chain is a stochastic process for which

$$P\left(X_{t_n}=Y_{i_n}\mid X_{t_{n-1}}=Y_{i_{n-1}},X_{t_{n-2}}=Y_{i_{n-2}},\ldots,X_{t_1}=Y_{i_1}\right)=P\left(X_{t_n}=Y_{i_n}\mid X_{t_{n-1}}=Y_{i_{n-1}}\right)\quad (X)$$

  for all n

  → a Markov chain has no memory of the earlier states

- The conditional probability (X) can be interpreted as the transition probability from state i to state j

$$W_{ij}=W\left(Y_i\to Y_j\right)=P\left(X_{t_n}=Y_j\mid X_{t_{n-1}}=Y_i\right)$$

Importance sampling Monte Carlo: Markov chain

- As usual for transition probabilities

$$W_{ij} \geq 0 \qquad \sum_j W_{ij} = 1$$

- Then, the total probability that at time t_n the system is in state Y_j is given by

$$P\left(X_{t_n} = Y_j\right) = \sum_i P\left(X_{t_n} = Y_j \mid X_{t_{n-1}} = Y_i\right) P\left(X_{t_{n-1}} = Y_i\right) = \sum_i W_{ij} P\left(X_{t_{n-1}} = Y_i\right)$$

- Consider time as a continuous rather than a discrete variable and write

$$P\left(X_{t_n} = Y_j\right) = P\left(Y_j, t\right)$$

Importance sampling Monte Carlo: Markov chain

- Master equation: A phenomenological set of first-order differential equations describing the time evolution of the probability of a system to occupy each one of a discrete set of states with regard to a continuous time variable

$\frac{dP}{dt} = AP$ where A is the matrix describing the transition rates

Importance sampling Monte Carlo: Markov chain

- During a Markov process, the time-dependent behavior of the probabilities is then given by the master equation

$$\frac{dP(Y_j,t)}{dt} = \sum_i W_{ij} P(Y_i,t) - \sum_i W_{ji} P(Y_j,t)$$

No memory of the past

- In equilibrium, there is a unique probability distribution $P_{\text{eq}}(Y_j,t)$ such that

$$\frac{dP_{\text{eq}}(Y_j,t)}{dt} = 0$$

Importance sampling Monte Carlo: Markov chain

- This is guaranteed by the detailed balance condition

$$W_{ji} P_{\text{eq}}(Y_j) = W_{ij} P_{\text{eq}}(Y_i)$$

- For a classical system in the canonical ensemble, the probability for the system to be in state i with energy E_i is given by $P_i = e^{-E_i/T} / Z$, where Z is the partition function
  - P is usually not known because in practice it is impossible to calculate Z for most systems

  → Use Markov chains

Importance sampling Monte Carlo: Markov chain

- We can generate each new state directly from the previous state. This can be easily done because we only need to consider the relative probabilities of two successive states i and j. From the detailed balance condition we get

$$\frac{W_{ji}}{W_{ij}} = \frac{P_j}{P_i} = e^{-(E_j - E_i)/T}$$

→ Only the energy difference $\Delta E = E_j - E_i$ needs to be known

Importance sampling Monte Carlo: Markov chain

- Any transition probability which satisfies the detailed balance condition is acceptable. The most widely used choice is the Metropolis form

$$W_{ij} = \begin{cases} e^{-\Delta E/T} & \text{if } \Delta E > 0 \\ 1 & \text{if } \Delta E \leq 0 \end{cases}$$

Importance sampling Monte Carlo: Metropolis Monte Carlo method

- Back to the 1D Ising model
- We use the MMC algorithm and the Monte Carlo sampling idea to write

$$U = \frac{\sum_{\{S_1,\ldots,S_N\}} E e^{-\beta E}}{\sum_{\{S_1,\ldots,S_N\}} e^{-\beta E}} = \sum_{\{S_1,\ldots,S_N\}} P(E)E \approx \frac{1}{\#\Omega} \sum_{\{S_1,\ldots,S_N\}\in\Omega} E(S_1,\ldots,S_N)$$

where Ω is the set of configurations generated by the MMC algorithm

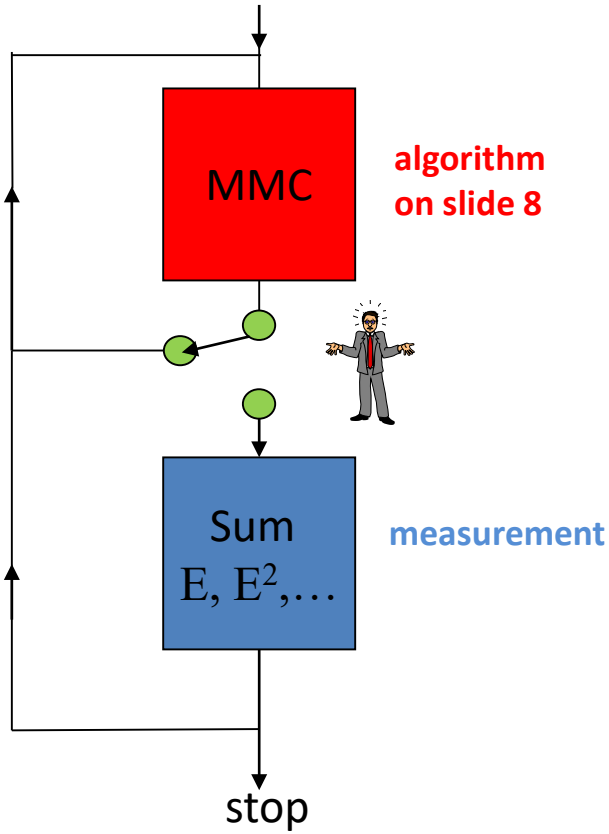
Importance sampling Monte Carlo: Metropolis Monte Carlo method

- In general, for any function $f(S_1,\ldots,S_N)$, its average F is given by

$$F = \frac{\sum_{\{S_1,\ldots,S_N\}} f(S_1,\ldots,S_N)e^{-\beta E}}{\sum_{\{S_1,\ldots,S_N\}} e^{-\beta E}} \approx \frac{1}{\#\Omega}\sum_{\{S_1,\ldots,S_N\}\in\Omega} f(S_1,\ldots,S_N)$$

Importance sampling Monte Carlo: Metropolis Monte Carlo method

- In practice
  1. perform N_{wait} MMC steps to let the system "relax" to the important states
  2. Perform N_{samples} MMC steps and take samples
- Typically $N_{\text{wait}} = N_{\text{samples}} / 10$
  (depends on parameters like temperature for example)



Switch open: relaxation (N_{wait} steps)
Switch closed: measurement (N_{samples} steps)

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.

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

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

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

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

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

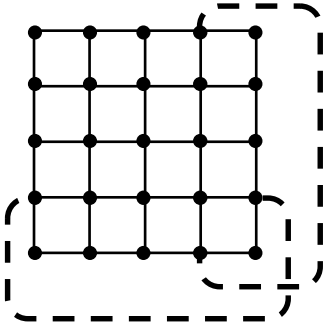
$$M/N^2 = \begin{cases} \left(1 - \sinh^{-4} 2\beta\right)^{1/8} & \text{if} \quad T < T_C = \dfrac{2}{\ln(1+\sqrt{2})} \\ 0 & \text{if} \quad T > T_C \end{cases}$$

Exercise:
1D and 2D Ising model

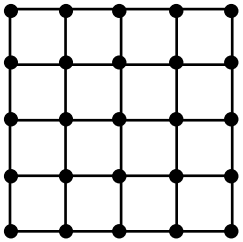
- 2D model: make 3 plots of the results of the average energy U/N^2, specific heat C/N^2 and magnetization M/N^2 per spin and put the data for $N = 10, 50, 100$ on the same plot
  - $N_{\text{samples}} = 1000, 10000$
- Interpret the results in terms of a phase transition from a state with magnetization 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 + 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 19, 2023