Exercises Monte-Carlo simulation I: Ising model

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Aufgabenstellung.

Main tasks

1. implementation of Metropolis algorithm for the two dimensional Ising model
2. determine the magnetization as a function of the temperature
3. localization of the phase transition according to the mag. susceptibility

Additional tasks:

1. determine further observables like U and C_V
2. determine correct error estimates using autocorrelation time
3. compare to the analytic predictions

In the following: A short summary from topics in the lecture.

The Ising model

- elementary magnets (spins $s_x \in -1, 1$) on a crystal lattice, first approximation: nearest neighbor interactions, cubic lattice

$$H(\{s_x\}) = -J \sum_{<x,y>} s_x s_y - h \sum_x s_x$$

$< x, y >$ all nearest neighbor pairs; h external magnetic field

- ferromagnetic interaction: $J > 0$
- magnetization in volume V:

$$M = \frac{1}{V} \sum_x s_x$$

Thermal averages

- thermal partition function ($\beta = 1/(k_B T)$)

$$Z(\beta) = \sum_{\{s_x\}} \exp(-\beta H)$$

- P probability for state $\{s_x\}$ in thermal ensemble

$$P(\{s_x\}, \beta) = \frac{1}{Z(\beta)} \exp(-\beta H(\{s_x\}))$$

- thermal average of M

$$\langle M \rangle(\beta) = \frac{1}{Z(\beta)} \sum_{\{s_x\}} M(\{s_x\}) \exp(-\beta H(\{s_x\}))$$

Monte-Carlo sampling

- importance sampling: good approximation from subset of configurations
- generate N configurations $(\{s_x\}_i)$ distributed according to P
- thermal average

$$\langle M\rangle(\beta) \approx \frac{1}{N}\sum_{i=1}^{N} M(\{s_x\}_i)$$

- use update process (Markov chain) to generate distribution $\{s_x\}_i \rightarrow \{s_x\}_{i+1}$

Update process

Main conditions for update algorithm

1. **ergodicity**
2. **detailed balance**: transition probability W of Monte-Carlo process

$$P(\{s_x\}_i)W(\{s_x\}_i, \{s_x\}_j) = P(\{s_x\}_j)W(\{s_x\}_j, \{s_x\}_i)$$

Detailed balance guarantees that the probability P is a fixed point of the process

$$\sum_{\{s_x\}_i} P(\{s_x\}_i)W(\{s_x\}_i, \{s_x\}_j) = \sum_{\{s_x\}_i} P(\{s_x\}_j)W(\{s_x\}_j, \{s_x\}_i) = P(\{s_x\}_j)$$

Metropolis update

- propose new configuration $\{s_x\}_j$ with trial probability $T(\{s_x\}_i, \{s_x\}_j)$
- accept with acceptance probability

$$A(\{s_x\}_i, \{s_x\}_j) = \min\left(\frac{P(\{s_x\}_j)T(\{s_x\}_j, \{s_x\}_i)}{P(\{s_x\}_i)T(\{s_x\}_i, \{s_x\}_j)}, 1\right)$$

- if rejected next configuration same as $\{s_x\}_i$

Proof simple:

$$P(\{s_x\}_i)T(\{s_x\}_i, \{s_x\}_j)A(\{s_x\}_i, \{s_x\}_j) \\ = P(\{s_x\}_j)T(\{s_x\}_j, \{s_x\}_i)A(\{s_x\}_j, \{s_x\}_i)$$

Single spin flip Metropolis update in Ising model

- $T(\{s_x\}_i, \{s_x\}_{i+1})$: single spin flip $s_x \to -s_x$
- microreversibility: $T(\{s_x\}_i, \{s_x\}_{i+1}) = T(\{s_x\}_{i+1}, \{s_x\}_i)$
- acceptance probability

$$A(\{s_x\}_i, \{s_x\}_{i+1}) = \min\left(\exp(-\beta\delta H), 1\right)$$

- difference depends only on local part

$$\delta H = H(\{s_x\}_{i+1}) - H(\{s_x\}_i) = H_x(\{s_x\}_{i+1}) - H_x(\{s_x\}_i)$$

- if rejected set $\{s_x\}_{i+1}$ to old configuration $\{s_x\}_i$

Observables and physics of the Ising model

- transition from high temperature disordered to low temperature ordered phase at T_c.
- low temperature: spontaneous magnetization $\langle M \rangle$.
- magnetic susceptibility $\chi_M = \frac{1}{V}(\langle M^2 \rangle - \langle M \rangle^2)$ has a peak at T_c

Further interesting observables:

- energy $\langle H \rangle$
- specific heat: $C_v = \frac{\beta^2}{V}(\langle E^2 \rangle - \langle E \rangle)$ (or derivative dE/dT)
- Binder cumulant: $U = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$
- correlation length

Error analysis

$$\langle M \rangle \approx \langle M \rangle_{MC} = \frac{1}{N} \sum_{i=1}^{N} M(\{s_x\}_i)$$

Naive error estimate:

$$\delta \langle M \rangle_{MC} = \sqrt{\frac{1}{N-1} \langle (M_i - \langle M \rangle_{MC})^2 \rangle_{MC}}$$

Two caveats:

1. simulations need equilibration in the beginning: Compare runs with complete up/down initial configuration.
2. consequent configurations not independent: Create averages of subsets of the data (binning) to have independent samples. Estimate the autocorrelation time τ

Autocorrelation

Autocorrelation function

$$C(t) = \frac{\frac{1}{N-t}\sum_{i}^{N-t}(M_i M_{i+t} - \langle M\rangle_{MC}^2)}{\langle M^2\rangle_{MC} - \langle M\rangle_{MC}^2} \sim e^{t/\tau_{exp}}$$

Integrated autocorrelation time

$$\tau_{int} = \frac{1}{2} + \sum_{t=1}^{\infty} C(t)$$

Ideally $\tau_{exp} \approx \tau_{int}$, real data $\tau_{int} < \tau_{exp}$

- plot τ_{int} as a function of summation length and check for plateau / maximum
- reasonable cut of sum: t with first negative value of $C(t)$

Hints for the implementation

- periodic boundary conditions are assumed
- one local update changes only spin at a single point; iteration through all lattice points x required
- one measurements after each iteration over complete lattice $\rightarrow$ average results for thermal average

Efficiency:

- local change of spin leads only to small change of H

$$\delta H = \delta H_x = -J \quad \delta s_x \sum_{y \in \text{up, down neighbors of } x} s_y$$

- $\delta s_x = (s_x)_{\text{new}} - (s_x)_{\text{old}} = -2(s_x)_{\text{old}} = 2(s_x)_{\text{new}}$ very simple for Ising model

Hints for the implementation of accept step

Probablility

$$A(\{s_x\}_i, \{s_x\}_{i+1}) = \min\left(\exp(-\beta\delta H), 1\right)$$

- choose random number r in interval $(0, 1]$
- calculate $h = \exp(-\beta\delta H)$
- accept if $r < h$, reject otherwise