Übungen zur Monte-Carlo-simulation I: Ising-Modell

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Aufgabenstellung.

Aufgaben

1. Implementieren Sie den Metropolis-Algorithmus für das zweidimensionale Ising-Modell.
2. Messen Sie die Magnetisierung als Funktion der Temperatur.
3. Lokalisieren Sie anhand der Daten für die Suszeptibilität den Phasenübergang.

Zusatz-Aufgaben

1. Bestimmen Sie die mittlere Energie und weitere Observablen.
2. Vergleichen Sie mit analytischen Formeln.
3. Berechnen Sie realistische Fehlerabschätzungen mit Hilfe der Autokorrelationszeit.

Im Folgenden sind eine kurze Zusammenfassung aus den Vorlesungen und Hinweise zur Lösung in englischer Sprache angefügt.

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 $\{s_x\}_i \to \{s_x\}_{i+1}$

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

$$\begin{aligned}\sum_{\{s_x\}_i} P(\{s_x\}_i)W(\{s_x\}_i, \{s_x\}_j) &= \sum_{\{s_x\}_i} P(\{s_x\}_j)W(\{s_x\}_j, \{s_x\}_i) \\ &= P(\{s_x\}_j)\end{aligned}$$

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