Optimized parallel tempering Monte Carlo

September 27, 2010 | Marco Müller
Overview

1 Introduction
   - The Ising Model
   - Fundamental Quantities in Statistical Physics

2 Monte Carlo Methods
   - Simple sampling
   - Importance sampling
   - Metropolis-Algorithm
   - Parallel Tempering

3 Results
Motivation

- (classical) Thermodynamics is well understood, lacks details
  - Out-of-equilibrium physics, structure formation?
  - Phase transitions?
  - Systems with $\approx 10^{23}$ particles
  - Known dynamics, but impractical to trace all particles

- Statistical Mechanics: approach by statistical methods
Ising Model

\[ \mathcal{H} = -J \sum_{\langle i,k \rangle} \delta_{s_i s_k} \quad s_i \in \{0, 1\} \]

- Many elementary magnets interacting with a coupling constant \( J \)
- Every magnet can be “up” or “down”
- Solved in 1d by [Ising, 1925]
- 2d-regular lattices:
  - Exact solution by [Onsager, 1944]
  - Exact calculation of the density of states for finite and periodic regular lattices by [Beale, 1996]
Phase transition

- Continuous phase transition at Curie-temperature $T_c$, classification by critical exponents

\[ \propto (1-T/T_C)^\beta \]

- Ferromagnetic: $m$ is preserved after an external field was removed
- Paramagnetic: $m = 0$, an external field is reinforced
Fundamental quantities

- Probability of finding a microstate with energy $E_i$ for a system in a heat bath with temperature $T$:

$$\mathcal{P}^B(E_i) \propto e^{-\frac{E_i}{k_B T}}$$

$$\beta := \frac{1}{k_B T}$$

- (canonical) partition function:

$$Z = \sum_{\{\text{all states}\}} e^{-\beta E_i} = \sum_i \Omega(E_i) e^{-\beta E_i}$$

$$\Omega(E_i) \ldots \text{density of states with energy } E_i$$
Exact enumeration

\[ Z = \sum_{\{\text{all states}\}} e^{-\beta E_i} \]

- Estimate for the 2d Ising magnet:
  - lattice size: \( L \times L = 10 \times 10 \)
  - number of states: \( 2^{L\times L} \approx 10^{30} \)
  - fast computer: \( 10^{-9} \text{s/spin-flip} \cdot 100 \text{ spins} \)
    \( 10^{-7} \text{s/configuration} \)

\[ \approx 10^{23} \text{s} \approx 10^{15} \text{y} \gg 10^{10} \text{y} \quad \text{age of the universe} \]

Better method?
Simple Sampling

\textbf{while not enough statistics do}

\textbf{for every spin in the system do}

\quad draw a random number \( r \in [0, 1) \);
\quad \textbf{if} \; r < 0.5 \; \textbf{then}
\quad \quad set spin 0
\quad \textbf{else}
\quad \quad set spin 1

\textbf{end}

\textbf{end}

measure energy;

\textbf{end}

\[ P^B(E_i) = \frac{1}{Z} e^{-\beta E_i} \]

\[ \text{Samples the disordered states } \beta = 0 \quad (T \to \infty) \]
Simple Sampling ($10^{11}$ samples)

\[ Z = \sum_i \Omega(E_i) e^{-\beta E_i} \]
Simple Sampling

while not enough statistics do
  for every spin in the system do
    draw a random number \( r \in [0, 1) \);
    if \( r < 0.5 \) then
      set spin 0
    else
      set spin 1
  end
end
measure energy;
Simple Sampling

```plaintext
while true do
    for every spin in the system do
        draw a random number \( r \in [0, 1) \);
        if \( r < 0.5 \) then
            set spin 0
        else
            set spin 1
        end
    end
    measure energy;
end
```
Importance Sampling

- Need for suitable algorithm to draw configurations according to their Boltzmann weight $\mathcal{P}^B$
- Set up a Markov chain

\[ \ldots \xrightarrow{p_{ij}} \{s_j\} \xrightarrow{p_{jk}} \{s_k\} \xrightarrow{p_{kl}} \ldots \]

- Allows to calculate expectation values as mean over a finite chain of length $N$

\[
\langle \mathcal{O} \rangle = \sum_{\{s_i\}} \mathcal{O}(\{s_i\})\mathcal{P}^B \approx \frac{1}{N} \sum_{j=1}^{N} \mathcal{O}(\{s_i\}_j)
\]
Metropolis Algorithm

- Update scheme for every system that allows the calculation of the energy of a state (discrete or continuous, short-range and long-range interactions, (off-)lattice, . . .)
- Proposed by [Metropolis et al., 1953]

\[
p_{ij} = \begin{cases} 
1 & E_j < E_i \\
\exp(-\beta(E_j - E_i)) & E_j \geq E_i
\end{cases}
\]
Metropolis Algorithm for spin models

initialize (system, initial state, geometry . . .);
while not having enough measurements do
  choose a spin;
  choose a new value for that spin;
  draw a random number \( r \in (0, 1] \);
  if \( r < p_{ij}^{\text{metr}} \) then
    accept new state;
  else
    reject new state;
  end
  if system in equilibrium;
  then
    measure observables;
  end
end
Parallel Tempering

- Problem: Application of Metropolis method extremely inefficient for systems exhibiting a particularly complex transition behaviour (e.g. spin glasses, proteins, ...)
- Improvements: cluster updates
- Generalized methods:
  - multicanonical sampling
    [Berg and Neuhaus, 1991]
  - Wang-Landau method
    [Wang and Landau, 2001]
  - parallel tempering
    [Swendsen and Wang, 1986], [Geyer, 1991],
    [Hukushima and Nemoto, 1996]
Parallel Tempering

- Basic idea: after local updates, update full configuration
Parallel Tempering

- Basic idea: after local updates, update full configuration

\[ \beta_0 \quad \beta_1 \quad \beta_2 \quad \beta_3 \quad \beta_4 \quad \beta_5 \quad \beta_6 \quad \beta_7 \quad \beta_8 \quad \beta_9 \]

- Metropolis criterion: valid updates with probability

\[ p_{ij}^{pt} = \min(1, e^{\Delta}) \quad \Delta = (\beta_j - \beta_i) [E_j - E_i] \]
Parallel Tempering

- Basic idea: after local updates, update full configuration

$$\beta_0 \quad \beta_1 \quad \beta_2 \quad \beta_3 \quad \beta_4 \quad \beta_5 \quad \beta_6 \quad \beta_7 \quad \beta_8 \quad \beta_9$$

- Metropolis criterion: valid updates with probability

$$p_{ij}^{pt} = \min(1, e^{\Delta}) \quad \Delta = (\beta_j - \beta_i) [E_j - E_i]$$
Parallel Implementation

- Exchange inverse temperatures instead of configurations
- Master-slave vs. exchange by each process
- Update attempts only on $(\beta\text{-})$-adjacent systems
First Results

- Verification by Jackknifing time series

Specific heat near the critical point of the 2d-Potts-Model, simulated using the Metropolis algorithm (left) and parallel tempering (right) with the following parameters: $q = 2$, grid dimensions $= 32 \times 32$, number of energies $= 2^{17}$, number of jackknife blocks $= 2^9$
First Results

- Verification with histogram-reweighting

Single histograms for 32 inverse temperatures (left) and density of states after Ferrenberg-Swendsen reweighting (right); parameters: $q = 2$, grid dimensions = $32 \times 32$, number of energies = $2^{20}$, number of jackknife blocks = $2^{12}$
Optimizations – $\beta$-Distribution

- Choosing the inverse temperatures:
  - with constant spacing
  - with constant overlap of the histograms

Single histograms for 32 inverse temperatures (left) and density of states after Ferrenberg-Swendsen reweighting (right); parameters: $q = 2$, grid dimensions $= 32 \times 32$, number of energies $= 2^{20}$, number of jackknife blocks $= 2^{12}$
Optimizations – $\beta$-Distribution

- $P(\beta_i, \beta_{i+1})$
- constant spacing
- constant overlap

- overlap($\beta_i, \beta_{i+1}$)

- heat bath

- constant spacing
- constant overlap

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Optimizations – $\beta$-Distribution
Achievements

- Development of parallel tempering Monte Carlo simulation in C++ using MPI
- \[ \mathcal{H} = - \sum_{<i,j>} J_{ij} \delta_{s_i s_j} \quad s_i \in \{0 \ldots q\} \]
- Hypercubic lattice with arbitrary dimensions
- configuration file for simulation parameters
- Surrounding Python scripts for data analysis, histogram reweighting, plotting
Future Plans

- Refinement of the beta distribution

\[
\beta_{\text{min}} \quad \square \quad \square \quad \square \quad \square \quad \square \quad \beta_{\text{max}}
\]

- Multiplexing

\[
\beta_{\text{min}} \quad \square \quad \square \quad \square \quad \square \quad \square \quad \beta_{\text{max}}
\]

- Multithreading on shared memory (GPGPU)
Further reading I

Exact distribution of energies in the two-dimensional Ising model.

Multicanonical algorithms for first order phase transitions.

Markov chain Monte Carlo maximum likelihood.

Exchange Monte Carlo method and application to spin glass simulations.

Beitrag zur theorie des ferromagnetismus.

Equation of state calculations by fast computing machines.
Further reading II


