Prof. Dr. W. Janke Heraeus Summerschool 2006

Monte Carlo Methods in Classical Statistical Physics

Assignments

1. **Exact enumeration and density of states**

   Compute the partition function of the one-dimensional Ising model with periodic boundary conditions by exact enumeration of all states for $L = 20$ spins ($2^L = 2^{20} \approx 10^6$ states) at $\beta J = 1$ (resp. $T = J/k_B$). Compare with the exact solution from a transfer-matrix calculation.

   How can the program be modified to obtain exact results for all temperatures? With a further small modification this can be generalized to all magnetic fields as well by counting the density of states $\Omega(E, M)$. Test your code again by comparing with exact results.

2. **Pseudo-random number generators**

   The generation of uniformly distributed pseudo-random numbers with a *Linear Congruential Generator* (LCG) uses the following rule:

   $$X_{i+1} = (aX_i + c) \bmod m,$$

   where their "quality" depends crucially on the choice of the parameters a, c, and m. Choose in the following the purposely non-optimal values $a = 5$, $c = 0$, $m = 2^{11} = 2048$, $X_0 = 1$.

   a) Implement this LCG with a normalization such that $X_i \in [0, 1)$.
   b) Plot the „time series " X_i of 10^4 random numbers and determine their period t_0.
   c) Measure the mean $\overline{X} = \sum_{i=1}^{N} X_i/N$ and variance $\hat{\sigma}_X^2 = \overline{X^2} - \overline{X}^2$ using $N = t_0$, $10\,t_0$, and $100\,t_0$ random numbers.

d) Plot the so-called *running average* $\overline{X}(n) = \sum_{i=1}^{n} X_i/n$ as function of n in the interval $n \in [30\,000, 40\,000]$.

e) Create a two-dimensional xy plot with $x = X_i$ and $y = X_{i+1}$ for $i = 1, 3, 5, \ldots$.

Use a more realistic LCG with larger period (e.g. *drand48*) to estimate the areas of a circle and ellipse by simple sampling (circle of radius $r = 1$ centered at $(1, 1)$ and analogously for the ellipse).

One method to generate Gaussian pseudo-random numbers is to first drawn two independent uniform pseudo-random numbers r_1 and r_2, and then to compute

$$x_1 = \sqrt{-2\ln r_1}\cos(2\pi r_2),$$

$$x_2 = \sqrt{-2\ln r_1}\sin(2\pi r_2),$$

which will be a pair of *independent* normal random deviates with mean zero and unit variance. Test this method by explicit simulation.

3. **Monte Carlo simulations of the 1D Ising model**

Write a Monte Carlo program for the simulation of the 1D Ising model with $L = 20$, 100, 1000 and 10000 spins and periodic boundary conditions using one of the local update algorithms:

a) Metropolis

b) Heat-bath

c) Glauber

Measure the energy, specific heat, magnetization and susceptibility for different temperatures ($k_BT/J = 0, \ldots, 1$) and compare with the enumeration results of assigment 1 and exact analytical results.

4. **Analyses of autocorrelations**

Write a computer program for the analysis of autocorrelations (autocorrelation function, integrated and exponential autocorrelation time). Test your program by means of the exact results given in the lecture for the bivariate Gaussian time series.

Compare your results with the binning method.

5. **Monte Carlo simulations of the 2D Ising model**

   Generalize your computer code of assignment 3 to the simulation of the 2D Ising model with periodic boundary conditions. Use square lattices of linear size $L = 4$, 8, 16, 32, 64, and 128 and compare for vanishing magnetic field in the range $k_BT/J = 0, \ldots, 1$ the energy and specific heat with exact results from the Kaufman solution [a useful reference is P.D. Beale, Phys. Rev. Lett. **76**, 78 (1996), which discusses a method for obtaining the density of states in 2D].

   Study the "finite-size scaling" behaviour close to the second-order phase transition at $K_c = J\beta_c = \ln(1+\sqrt{2})/2 \approx 0.44$ and determine the critical exponent ratios α/ν, β/ν, and γ/ν from fits to the respective power laws.

   Study the growth of autocorrelations with system size using the methods of assignment 4.

6. **Single-cluster algorithm for the 2D Ising model**

   Implement the (non-local) Wolff single-cluster algorithm for the 2D Ising model. Test your program by comparison with the numerical results of assigment 5 and the exact analytical solution. Estimate close to criticality the performance by measuring the autocorrelation time.

   Verify that the average (Fortuin-Kasteleyn) cluster size is an estimator for the (reduced) susceptibility $\chi' = L^2\langle m^2\rangle \propto L^{\gamma/\nu}$.

   What do you find for the finite-size scaling of the average *geometric* cluster size (which can be easily recorded in the same simulation run)?

7. **Single-histogram reweighting**

   Perform one simulation of the 2D Ising model (with periodic boundary conditions) on a 16^2 lattice at $J\beta_c \approx 0.440\,686$ ($\beta = 1/k_BT$). Construct from the time-series data for E and M the energy histogram and determine the reweighted distributions at $J\beta_1 = 0.375$ and $J\beta_2 = 0.475$. Compare with Beale's exact results or independent simulations at these temperatures. Analyze the quality of the reweighted histograms critically.