Exercises for the lecture

Fundamentals of Simulation Methods

WS 2015/16

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Exercise sheet 10 ***(due date: Jan 22, 2016, 11am)***

Sampling Techniques and Monte Carlo Simulation

1) Rejection method

We would like to produce a random sample $\{x_i\}$ drawn from the probability distribution function (PDF)

$$p(x) = \frac{p_0}{(x-2)^4 + \sin^8(x-3)}, \tag{1}$$

for $0 \leq x < 5$, with $p(x) = 0$ outside of this interval.

(a) Determine p_0 such that the function is normalized, i.e.

$$\int_0^5 p(x)\,\mathrm{d}x = 1. \tag{2}$$

(b) Use the rejection method with a uniform parent distribution over the interval $0 \leq x < 5$ to create a sample of $N = 10^6$ numbers from this distribution. What is the rejection rate? Plot a histogram of the distribution of your points, using 100 bins with a width $\Delta x = 0.05$, and compare it with the target distribution function on a common plot with logarithmic y-axis.

(c) Now consider a function $f(x)$ meant to provide an envelope for $p(x)$. Confirm that the piecewise linear

$$f(x) = \frac{y_{n+1} - y_n}{x_{n+1} - x_n}(x - x_n) + y_n \quad \text{for } x_n \leq x \leq x_{n+1}, \tag{3}$$

with $n \in \{0, 1, 2, 3, 4\}$ fulfills $p(x) \leq f(x)$ over the interval $[0, 5]$ for the points $(x_0, y_0) = (0, 0.01)$, $(x_1, y_2) = (1.8, 0.15)$, $(x_2, y_2) = (2.35, 2.5)$, $(x_3, y_3) = (3.0, 0.1)$, and $(x_4, y_4) = (5.0, 0.002)$. Use $f(x)$ as an auxiliary function in the rejection method to more efficiently sample the function $p(x)$. What is the rejection rate now? Verify with another histogram plot that the obtained sample is correct.

2) Sampling a given distribution with a Monte Carlo Markov chain

Let's assume we want to generate random numbers from the distribution

$$p(x) \propto \exp\left(-\left[x + 2\cos^2(x)\right]^2\right). \tag{4}$$

This simple case could also be done with the rejection method, but here we want to adopt a different approach, namely the use of a stochastic process constructed with the Metropolis algorithm.

(a) Start with some random guess x_0 for which $p(x)$ is not zero.

(b) Make a proposal for x_i' in your chain by adding a random number drawn uniformly from the interval $[-1, 1]$ to x_{i-1}.

(c) Accept the proposal with probability

$$r = \min\left(1, \frac{p(x_i')}{p(x_{i-1})}\right), \tag{5}$$

i.e. in the case of acceptance make it the entry x_i in your Monte Carlo chain. Otherwise, adopt the unmodified x_{i-1} as your element x_i. Then proceed with the next element $i+1$.

(d) Produce a chain with $N = 10^6$ elements, and make a histogram with bin size $\Delta x = 0.02$ of the entries in order to verify that they correctly sample the overplotted shape of $p(x)$. How many *different* points are in your chain?

3) Monte Carlo simulation of the 2D Ising model

We consider a 2D Ising model with the partition function

$$Z = \sum_{\{s_x=\pm1\}} \exp\left[-\frac{\beta}{2} \sum_{\text{ngbs of } y} (1 - s_x s_y)\right] \tag{6}$$

for spins with values $s_x = \pm1$ on a regular lattice of Cartesian topology. For every latice site x, the interaction term only involves the four nearest neighbours y on adjacent lattice sites. Use a $N = 32^2$ lattice with periodic boundary conditions.

We have the goal to measure the average magnetization

$$\langle |M| \rangle = \left\langle \left| \frac{1}{N} \sum_x s_x \right| \right\rangle \tag{7}$$

in thermal equilibrium for different values of β, namely $\beta = 1.6$, 1.3, 1.1, 1.0, 0.9, 0.8, 0.7, 0.6, 0.4, 0.1.

(a) For each value of β, go through the lattice in red-black order for at least 3000 times to establish thermalization. At each encountered lattice site x, calculate the interaction energies E_+ and E_- for the spin up and the spin down directions of x, respectively. Then choose for the site the spin-up direction with the *heat bath* (Gibbs sampling) probability

$$p_+ = \frac{\exp(-E_+)}{\exp(-E_+) + \exp(-E_-)}, \tag{8}$$

and the spin-down direction correspondingly with probability $p_- = 1 - p_+$.

(b) After the thermalization period, take measurements of M after at least 1000 full mesh sweeps and calculate the average $\langle |M| \rangle$. Report this in a table for each β.

(c) Plot $\langle |M| \rangle$ as a function of $T \propto 1/\beta$. We note that this model has a phase transition at a critical $\beta_c = \log(1 + \sqrt{2}) = 0.881$ (corresponding to a critical temperature $T_c \propto 1/\beta_c$). Below this temperature (i.e. for $\beta > \beta_c$), the systems shows spontaneous magnetization. The present 2D model without external field has been solved analytically by Onsager. In 3D, no analytic solution is known but it can be readily obtained with Monte Carlo simulations.