Problem sheet 2

1. Hyperplanes in pseudo-random numbers

Generate a three- and a two-dimensional plot of points (s_n, s_{n+1}, s_{n+2}) and (s_n, s_{n+1}) taken from the multiplicative linear congruential generator $a = 137$, $c = 187$ and $m = 256$.

2. Out of luck in Monte Carlo

We are interested in the integral

$$I = 2 \int_0^1 dx \int_0^1 dy \int_0^1 dz \, \sin^2 \left(2\pi (9x - 6y + z) \right).$$

This integral can be solved analytically by doing the z-integration first and yields 1. Suppose we are ignorant about this possibility and perform a brute-force Monte Carlo integration using the multiplicative linear congruential generator $a = 65539$, $c = 0$ and $m = 2^{31}$. Innocent as we are we use three consecutive random numbers from the generator to define a point in the cube: $(x, y, z)_n = (s_{3n}/m, s_{3n+1}/m, s_{3n+2}/m)$. What do you get ? In order to see what went wrong show that three consecutive numbers of this generator satisfy

$$(9s_n - 6s_{n+1} + s_{n+2}) \mod m = 0.$$

Instead of $m = 2^{31}$ you might also take $m = 2^{29}$. To check the implementation of your generator: The first few random numbers obtained from the seed $s_0 = 1$ are: 0.0001220759004, 0.0007324386388, 0.003295948729, 0.01318374462, 0.04943892919, 0.1779798735, 0.6229288783, 0.1357544083, 0.2081665453 for $m = 2^{29}$.
For $m = 2^{31}$ the sequence starts with 0.00003051897511, 0.0001831096597, 0.0008239871822, 0.003295936156, 0.01235973230, 0.04449496837, 0.1557322196, 0.5339386021, 0.8020416363 0.006802399177.

3. The Ising model

The Hamiltonian of the Ising model is given by

$$H_{Ising} = -J \sum_{\langle i,j \rangle} S_i S_j,$$

where $J > 0$ is a constant, $\langle i, j \rangle$ denotes the sum over all next-neighbours and the spin S_i at site i takes the values ± 1. Observables are given by

$$\langle O \rangle = \frac{\sum O(\phi) e^{-H(\phi)/kT}}{\sum e^{-H(\phi)/kT}},$$

where the sum runs over all possible states. One observable is the magnetization M or the order parameter. For the Ising model the magnetization is given by

$$M_{Ising} = \frac{1}{N} \sum S_i$$

Write a Monte Carlo program which simulates the two-dimensional Ising model on a 16×16 lattice with periodic boundary conditions using the Metropolis algorithm. (Note that with a 16×16 lattice, the total number of states is 2^{256}. This is far too large to evaluate the partition sum by brute force.) You may initialize the model with all spins up (cold start) or with a random distribution of spins (hot start). Step through the 256 spins one at a time making an attempt to flip the current spin. Plot the absolute value of the magnetization for various values of $K = J/kT$ between 0 and 1. Is anything happening around $K = 0.44$?