Simulation methods in physics

Homework 2
Return before 13.00 on Tue 25.2., to Ari Hietanen's mailbox (C-wing 3rd floor), or by e-mail ari.hietanen@helsinki.fi

1. Let us do one realistic case of non-trivial Monte Carlo integrations. The following 8-dim. "twisted H" integral appears at 4-loop level in perturbation theory (appeared in Aleksi Vuorinen's pro gradu):

$$\int_0^1 d^8\vec{x}\ f(\vec{x})$$

where the function

$$\begin{aligned} f(\vec{x}) &= \frac{1}{8\pi^2}\frac{y_1^{9/2}A^{3/2}}{[(AC-E^2)(AB-D^2)-(AF-DE)^2]^{3/2}} \qquad \text{if } \sum_{i=1}^{8} x_i \le 1 \\ f(\vec{x}) &= 0 \qquad \text{otherwise.} \end{aligned}$$

Here

$$\begin{aligned} s &= 1-\textstyle\sum_{i=1}^{8} x_i \\ y_1 &= x_1+x_5+x_6+s \\ y_2 &= x_2+x_7+x_8+s \\ y_3 &= x_3+x_5+x_7+s \\ y_4 &= x_4+x_6+x_8+s \\ A &= y_1y_2-s^2 \\ B &= y_1y_3-(x_5+s)^2 \\ C &= y_1y_4-(x_6+s)^2 \\ D &= y_1(x_7+s)-s(x_5+s) \\ E &= y_1(x_8+s)-s(x_6+s) \\ F &= y_1s-(x_5+s)(x_6+s) \end{aligned}$$

The function is lengthy but straightforward to program. Aleksi tells that it took 2 days for Mathematica to evaluate this to 1 (slightly incorrect) digit.

A) Calculate the integral using standard uniform sampling (one significant digit is enough). Note that the integrand is zero except in the corner $\sum_{i=1}^{8} x_i < 1$. During the integration, measure also the hit rate on this corner – i.e. the fraction of points which hit it. This gives the estimate of the volume of the corner.

Note that the hit rate is quite small, so you need quite a few points to get a result.

B) Now use importance sampling: choose each component x_i with probability $p(x_i) = 2(1-x_i)$. Thus, the full probability of vector $\vec{x}$ is $p(\vec{x}) = \prod_i p(x_i)$. What is the hit rate now? Calculate the integral to 2 significant digits.

Hint: now you can "invert" each component of x_i separately, which is pretty straightforward.

As a check, the order of magnitude of the integral is ~ 0.0001.

2. Make a 2-dimensional Ising model Monte Carlo simulation program which uses *heat bath* to update the spins. The partition function of the model is ($s_x = \pm 1$)

$$Z = \sum_{\{s_x=\pm 1\}} \exp\left[-\frac{\beta}{2}\sum_{<xy>}(1 - s_x s_y)\right].$$

(in the literature the Ising model is often defined without the factor 1/2 in β. Multiply values by that for comparison).

Measure the average magnetization

$$\langle |M| \rangle = \langle \left| \frac{1}{V} \sum_x s_x \right| \rangle$$

at $\beta = 1.6,\ 1.3,\ 1.0,\ 0.8,\ 0.6,\ 0.4$. Use a 32^2 lattice, and

1. Thermalize (at least) for first 5000 full lattice update sweeps before starting the measurements

2. Do at least 40000 measurements for each β.

Give the result with error estimates; in this case, you can use the naive error estimate (i.e. assume that each measurement is statistically independent).

This is an important problem: this program will be used in many future homework exercises!

For ease of the modification, do not hard-code the lattice size or the coupling β. Use (for example) the constant definitions

`#define nx 32` in C, or

`parameter(nx = 32)` in Fortran.