Monte Carlo simulation methods **Homework 4, 29.11.2007**

Return the solutions (with program printouts) at the latest at the beginning of the 29.11. excercise session. You can also e-mail the solutions to Ahti Leppänen, <ahtilepp AT mail.student.oulu.fi>.

1. Let us assume that we have 2 independent random variables x and y, which are distributed according to gaussian distributions of mean $\bar{x}$ and $\bar{y}$ and variance σ_x and σ_y, respectively (that is, $p(x) \propto \exp[-(x-\bar{x})^2/2\sigma_x^2]$).

   Show, by direct calculation, that the sum $z = x+y$ also is distributed according to gaussian distribution, with mean $\bar{z} = \bar{x} + \bar{y}$ and variance $\sigma_z = \sqrt{\sigma_x^2 + \sigma_y^2}$.

2. Consider the 3-state Potts model from homework 3. Make a simulation at the critical inverse temperature $\beta = \ln(1+\sqrt{3})$ using a system of size 64^2, and measure the energy

$$E = \sum_{<i,j>} [1 - \delta(s_i, s_j)]$$

   and the absolute (total) magnetisation

$$|M| = \frac{3}{2}\left[\max(M_1, M_2, M_3) - \frac{V}{3}\right], \qquad \text{where} \quad M_s = \sum_i \delta(s, s_i)\,.$$

   Do at least $\sim$ 50 000–100 000 measurements.

   a) From these measurements calculate (with errors!) $\langle E \rangle$, $\langle |M| \rangle$, and the sum and difference $\langle E + |M| \rangle$ and $\langle E - |M| \rangle$. What the errors in the sum and difference would be if E and $|M|$ were independent random variables?

   b) Calculate the magnetic susceptibility $\chi_M = \frac{1}{V}(\langle |M|^2 \rangle - \langle |M| \rangle^2)$ and reweight it in β in a narrow range around the simulation β, using, say, 10–20 values of β so that you can find the local maximum. Repeat this analysis using volumes 16^2 and 32^2, and plot the results. *Qualitatively* describe the location and value of the maximum (compare with the Ising model result in Sec. 9.2)

      For simplicity you can ignore the error analysis in this case (though for any realistic results error analysis would be necessary!) You do not need to locate the maxima precisely, just a qualitative description is sufficient (no fits etc.).

      Note that you need to reweight separately $|M|$ and $|M|^2$.

   Hints:

   In order to calculate the sums and differences in a) or the quantities needed for reweighting in b), you can make small modifications to the `errors.c` program. Original data has been read in after the call to `readdata`, and it is thus available for further modifications.

   Another simple way is to use standard UNIX utilities like `awk`. For example, if file1 contains measurements of (at least) 3 quantities on a line, command

   ```
   awk '{ print $2 + $3, $2 - $3 }' file1 > file2
   ```

   prints out the sum and difference of the 2nd and 3rd to file file2.