Homework 1 (CSM1)

Due: April 18, 2016.

The purpose of these exercises is that of learning to treat numerical data that have been generated in Monte Carlo or Molecular Dynamics simulations.

DATA SETS: Four data files are provided: `data1.txt`, `data2.txt`, `data3.txt`, and `datablocked.txt`. On each line of the first two files, there are three numbers: the first number is the Monte Carlo time, the second number and third number correspond to measurements. U_1 and U_2 are the two quantities reported in `data1.txt` (second and third column, resp.) and U_3 and U_4 are the two quantities reported in `data2.txt`. File `data3.txt` provides U_5. File `datablocked.txt` contains blocked variables that will be used below: we give on each group of 5 subsequent lines, the block number and the average value of the five observables.
Data in: `http://elearning2.uniroma1.it/course/view.php?id=2878`

Data are thermalized: check by looking at $U_i(t)$ versus Monte Carlo time t.

- **Blocking analysis**. First, compute the average and error on $\langle U_i \rangle$ neglecting correlations, i.e., assuming that data are independent.

  Second, generate blocked data. If $U_i(t)$, $t = 1, 60000$ are the original data define

  $$U^{(1)}(t) = \frac{1}{2}[U_i(2t-1) + U_i(2t)]$$

  $$U^{(k)}(t) = \frac{1}{2}[U_i^{(k-1)}(2t-1) + U_i^{(k-1)}(2t)]$$

  Compute average and error on the blocked variables for increasing values of k till the error stabilizes.

  Repeat the analysis for all five observables U_1, U_2, ...

- **Autocorrelation analysis**. Compute the autocorrelation function for the five observables and the corresponding integrated autocorrelation time. Use the estimates of the autocorrelation times to estimate the error on the sample means of U_i. Compare the results with those obtained in the blocking analysis.

- **Jackknife**. Consider the blocked variables with blocks of length 2500. They are provided in file `datablocked.txt`, which contains all five quantities together. They can be considered as essentially independent (is this consistent with previous results?). Define ($i = 2, 3, 4, 5$)

  $$R_i = \frac{\langle U_i \rangle}{\langle U_1 \rangle}.$$

  Compute R_i and its error using the jackknife method. Compare the error with those obtained by using the independent-error formula and the worst-error formula (use the errors computed with the autocorrelation analysis).