

Homework 1 (CSM1)

Due: April 21, 2017.

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: Two data files are provided: `data1.txt`, `data2.txt`. On each line 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`.

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 .

- 1) **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 $U_i(t)$, $t = 1, 100000$ 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 four observables U_1, U_2, \dots . Show your results for the error in a graph (error versus k) and report in a table the best estimate of the error for each observable.

- 2) **Autocorrelation analysis.** Compute the autocorrelation function for the four observables and the corresponding integrated autocorrelation time (report τ_{int} in a table for each observable). Use the estimates of the autocorrelation times to estimate the error on the sample mean of U_i . Compare the results with those obtained in the blocking analysis (report the results for the error in the same table).
- 3) **Jackknife.** Generate blocked variables with blocks of length 2000. They can be considered as essentially independent (is this consistent with previous results?). Define ($i = 2, 3, 4$)

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

Compute R_i and its error using the jackknife method applied to the blocked variables. 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). Present the three different estimates in a table.