

Homework 1 (CSM1)

Due: April 25, 2021

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

1) **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 . Repeat the analysis for all four observables U_1, U_2, \dots

2) **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 $U_i(t)$, $t = 1, 200000$ 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 (again, assuming that data are independent) on the blocked variables for increasing values of k till the error stabilizes.

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. Compare the results with those obtained using the autocorrelation function (report the results for the error in the same table).

3) **Improved blocking analysis.** Repeat the computation using the improved blocking method. Show your results for the error in a graph (error versus k) and report the final estimate of the error in the same table as before.

4) **Jackknife.** Generate blocked variables with blocks of length 2500. 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.