

Exercises 1 (CSM1)

Due: April 13, 2015.

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 `databloked.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 `databloked.txt` contains blocked variables that will be used below.

- **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 $U_i(t)$, $t = 1, 25000$ 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, \dots

- **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.
- **Functions of mean values.** Define ($i = 2, 3, 4, 5$)

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

Compute the error by using the independent error formula and by taking into account the correlations between numerator and denominator (for this purpose one can perform a blocking analysis of a properly defined quantity, or an autocorrelation analysis of the same quantity).

Repeat the analysis for all four observables U_2, U_3, \dots

- **Jackknife.** Consider the blocked variables with blocks of length 1000. They are provided in file `databloked.txt`, which contains all five quantities together. They can be considered as essentially independent (is this consistent with previous results?). Compute R_i using the jackknife method. In particular, determine the bias and the error. Compare with the analyses performed above.