

# Worksheet 7: Error Analysis

May 21, 2014

## General Remarks

- The deadline for the worksheets is **Wednesday, 21 May 2014, 10:00** for the tutorial on Friday and **Friday, 23 May 2014, 10:00** for the tutorials on Tuesday and Wednesday.
- On this worksheet, you can achieve a maximum of 10 points.
- To hand in your solutions, send an email to
  - Johannes (zeman@icp.uni-stuttgart.de; Tuesday, 9:45–11:15)
  - Tobias (richter@icp.uni-stuttgart.de; Wednesday, 15:45–17:15)
  - Shervin (shervin@icp.uni-stuttgart.de; Friday, 11:30–13:00)

the data needed in this worksheet can be found in the file `ws7.pkl.gz` on the home page.

## Task 7.1: Error Analysis and the Autocorrelation Function (4 points)

The file `artificial.npy` contains five (artificially generated) time series with a well-defined autocorrelation time. To read the data from the file, use the following command:

```
d0, d1, d2, d3, d4 = numpy.load('artificial.npy')
```

- **7.1.1** (2 points) Compute and plot the interesting parts of the autocorrelation functions of the different time series.
- **7.1.2** (1 point) Estimate the autocorrelation time  $\tau_C$  of the different series from the plots, by fitting the corresponding exponential function to the autocorrelation function. You can do this either visually (*i.e.* by trying out different values of  $\tau_C$  and see how it fits) or by any other method (*e.g.* `scipy.optimize.curve_fit()`).
- **7.1.3** (1 point) Compute the mean values of the different series and their statistical errors from the estimated correlation times.

## Hints

- You may want to use the functions `numpy.mean()`, `numpy.std()` or `numpy.var()`.
- The autocorrelation function will not converge towards 0 when the mean value of the functions does not converge to 0.
- The autocorrelation function decays very quickly, so you will have to zoom the function at small  $\tau$ .
- When fitting the exponential, you should only fit at small  $\tau$ .

## Task 7.2: Error Analysis of Real Simulation Data (2 points)

As in the previous worksheet, the file `simulation.npy` contains data of an actual Molecular Dynamics simulation of a charged colloidal particle (Charge +300, Radius 50 nm) in a solution of monovalent and multivalent ions (Charges  $-1$ ,  $+1$  and  $-3$ ).

To read the data from the file, use the following command:

```
t, n1, n2, n3 = numpy.load('simulation.npy')
```

In the previous worksheet, you have determined the equilibration time of the time series. In all of the following tasks, use only the data *after* the equilibration time (*i.e.* the *equilibrated* data).

- **7.2.1** (1 point) qPlot the interesting parts of the autocorrelation function of the equilibrated data.
- **7.2.2** (1 point) As in the previous task, estimate the mean values, the statistical errors and the correlation times of the equilibrated data.

## Task 7.3: Binning Analysis (4 points)

- **7.3.1** (2 points) Implement a Python function that computes the binning error estimate for a given bin size of a given data set.
- **7.3.2** (1 point) Plot the binning error estimate versus the bin size for the different data sets (both the artificial and the simulation data) and read off the binning error estimates and the correlation times.
- **7.3.3** (1 point) Compare the binning autocorrelation times with the estimated autocorrelation times from tasks 6.1 and 6.2. Do they match? Which of them do not match? Do you have an idea why?