

Modelling Biochemical Reaction Networks

Lecture 15: Analyzing stochastic simulations

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*What information can we get
from stochastic simulations?
Evolution in time of probability distribution*

- ▶ Carry out lots (usually thousands) of stochastic simulations from identical initial conditions.
- ▶ Sample at regular intervals and calculate statistics for the number of molecules of each type (e.g. open channels in the model previously studied) across all the simulations.
- ▶ Can be done in `xppaut` using pseudo-arrays
 - ▶ Special notation for lists of propensities in `gill()` function: `a{1-100}`.

*What information can we get
from stochastic simulations?
Stationary probability distribution*

- ▶ Instead of averaging across simulations, get a time average from one long simulation, perhaps after discarding an initial transient.
- ▶ The distribution is stationary if we get the same distribution (same statistical properties) when we (e.g.) double the simulation time.
- ▶ Can do some of this work in xppaut, but a spreadsheet is often more convenient

Checking for stationarity

- ▶ Get a long time series, discarding any visually obvious initial transients.
- ▶ Split the time series in two.
- ▶ Calculate the average and its standard error for one of the variables (e.g. N_O) for each half of the time series.
 - ▶ Standard error of the mean: σ/\sqrt{N} , where σ is the standard deviation, and N is the number of samples
- ▶ If the two averages are within one standard error of each other, the time series is likely stationary.
- ▶ Once a time series has been determined to be stationary, analyze the whole data set