

Project III 2022/23

Stochastic Kinetic Models

A stochastic kinetic model (SKM) typically refers to a reaction network, an associated rate law and a probabilistic description of the reaction dynamics. They are increasingly used to account for the inherent stochasticity exhibited by interacting populations of species in areas such as epidemiology, population ecology and systems biology.

A Markov jump process (MJP) provides the most natural description of the time-course behaviour of the species involved in the reaction network. In scenarios where species numbers can be reasonably regarded as continuous, it is commonplace to approximate the MJP to give an Itô stochastic differential equation known as the chemical Langevin equation (CLE). In order to test hypotheses *in-silico*, plausible parameter values must be obtained given data at discrete times, that may be incomplete (in the sense of information on a subset of species in the reaction network) and subject to error. This setting, when combined with either the MJP or CLE modelling framework precludes straightforward likelihood-based inference owing to the intractability of the observed data likelihood.

This project will allow students to get to grips with the various SKM representations and their associated simulation algorithms, which will allow visualisation of the dynamics of various systems of interest, selected from the above application areas. The project will then consider the inference problem, within a Bayesian setting. That is, given data at discrete times, what are the parameter values that are consistent with the data? This will involve constructing Markov chain Monte Carlo schemes for posterior exploration, applied to some simple SKMs.

Prerequisites: Markov chains II, Probability II, familiarity with the statistical language R

Corequisites: Bayesian Computation and Modelling III

Resources (indicative)

- Try searching for "The Gillespie algorithm" which is a simulation algorithm for generating draws of the most natural MJP representation.
- Book chapter on SKMs and accompanying R code:
<https://github.com/csgillespie/In-silico-Systems-Biology>
- Allen, L. S. (2003). Stochastic Processes with applications to Biology. Pearson Prentice Hall.
- Wilkinson, D. J. (2019). Stochastic modelling for Systems Biology. CRC Press 3rd Edn.
<https://darrenjw.github.io/work/smfsb/3e/>

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