Project III 2024/25

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 epidemics, 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 Ito stochastic differential equation (SDE) known as the chemical Langevin equation (CLE). Although it is not usually possible to solve this SDE, it can be linearised to give a tractable approximation.

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.

Essential companion modules: Bayesian Computation and Modelling III

Resources (indicative)

- <u>Book chapter</u> on SKMs and accompanying <u>R code</u>.
- 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/

Anticipated outcomes

- A literature review, outlining existing approaches to simulating stochastic kinetic models.
- A discussion of existing approaches to Bayesian inference for SKMs.
- Focus on one or more inference techniques with application to real or synthetic data.
- A suite of bespoke R functions for simulating and fitting SKMs.

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