Project III 2026/27

Stochastic Kinetic Models

Supervisor: Andrew Golightly
Project research area: Statistics

Background

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 (e.g. to describe interactions between susceptible, infected and recovered individuals), population ecology (e.g. to describe predator-prey interactions) and computational biology (e.g. to model the dynamics of the components of some intra-cellular process).

A Markov jump process (MJP) is a continuous-time, discrete-valued stochastic process that satisfies the Markov property. Intuitively, the process jumps from one discrete state to another after an exponentially distributed time period. Importantly, an MJP provides the most natural description of the time-course behaviour of the species involved in the reaction network. Exact simulation of an MJP is straightforward via Gillespie's direct method (see Figure 1), albeit computationally intensive, due to capturing all reaction times and types. Consequently, various approximations of the MJP have been developed, including tau leaping (where numbers of reaction events over a time interval of length tau are approximated via a Poisson distribution) and the chemical Langevin equation (which models species dynamics via a stochastic differential equation).

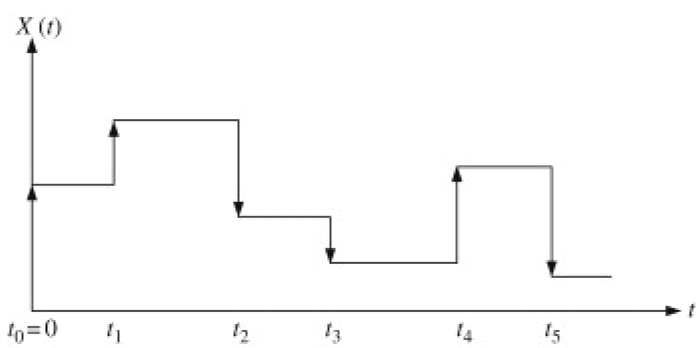

Figure 1: Markov jump process illustration (source: Ible, O. C. (2013), *Markov processes for stochastic modelling*).

This project will allow students to get to grips with the theory and methods underpinning various SKM representations and their associated simulation algorithms, which will allow visualisation of the dynamics of a range of systems of interest, selected from application areas in epidemiology, population ecology and computational biology. The individual project will then consider the inference problem, within a Bayesian setting. That is, given data at discrete times, one must determine the parameter values that are consistent with the data. This will involve construct simulation-based schemes, such as Markov chain Monte Carlo (MCMC), for posterior exploration, applied to some simple SKMs.

Group Project

The group project will involve learning about the mathematical formulation and properties of Markov jump processes and their approximations, and implementing bespoke R code for their simulation.

By the end of the group project, you will have an understanding of:

- The poisson process (definition, properties, simulation).
- Markov jump processes (definitions, properties, simulation algorithms).
- Approximations of Markov jump processes (definitions, properties, simulation algorithms).
- Specific examples in areas including epidemiology, population ecology, computational biology).

By the end of the group project, you will be able to:

- Understand the theoretical underpinnings and properties of MJPs.
- Write R code to simulate from MJPs using Gillespie’s direct method.
- Write R code to simulate from various approximations of a given MJP.
- Compare and contrast simulation approaches, both in terms of accuracy and efficiency.

Mode of operation in evidence of learning

The project will involve learning through reading and programming in R. Students will demonstrate their understanding by comparing theory to simulation results, writing R code to implement core methodology, analysing simulated and real data sets, and clearly communicating the material in both written and oral formats.

Individual Project

The individual project will involve learning about Bayesian approaches to inference for Markov jump processes and their approximations, and implementing bespoke R code for posterior simulation.

By the end of the individual project, you will have an understanding of:

- The challenges for performing Bayesian inference for MJPs and their approximations.
- Metropolis-Hastings for simple MJPs and deterministic approximations.
- Various approximate Bayesian computation schemes and their application to MJPs and approximate models thereof.
- The challenges and limitations of these inference methodologies in real world settings.

By the end of the individual project, you will be able to:

- Discuss existing approaches to Bayesian inference for MJPs and their approximations.
- Write a suite of bespoke R functions for fitting MJPs and their approximations.
- Apply Bayesian inference techniques to real and/or synthetic data.
- Compare and contrast inference approaches in terms of efficiency.
- Interpret your results.

Mode of operation in evidence of learning

The project will involve learning through reading and programming in R. Students will demonstrate their understanding by comparing theory to simulation results, writing R code to implement core methodology, analysing simulated and real data sets, and clearly communicating the material in both written and oral formats.

Essential co-requisite: MATH3421 Bayesian Computation and Modelling III

Resources (indicative)

- Book chapter on SKMs and accompanying R code.
- 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/

Additional information: contact Andy Golightly (andrew.golightly@durham.ac.uk)