MA30257/MA50257- Methods for stochastic systems coursework

Date Set: Wednesday 8th November, 2023.

Deadline for submission of answer document: Noon, Friday 8th December, 2023.

Marks: This coursework will account for 25% of the total marks of the unit for both MA30257 and MA50257. The marks available for each question are in square brackets at the end of the question.

Feedback: An annotated copy of the completed coursework will be returned within three weeks of the deadline.

Artificial intelligence: The use of generative artificial intelligence (AI) in this task is strictly prohibited. Any student found to have employed AI as part of this coursework will receive a score of zero.

Objective: Answer the questions below including writing code to reproduce the requested figures. Where appropriate give numerical answers correct to one decimal place.

Consider chemical species A in a container of volume ν subject to the following four chemical reactions

$$A + A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} A \quad A \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} \phi. \tag{1}$$

In your simulations use the following parameter values (these can be kept general in your analytical workings)

$$k_1/\nu = 0.1, \quad k_{-1} = 1, \quad k_2 = 0.1 \quad \text{and} \quad k_{-2}\nu = 1,$$

where the parameters are in terms of reactions per arbitrary time unit. The system is initiated with $N = 1$ particle.

Question 1 Write down the probability master equation for $p_n(t)$, the probability of there being n particles at time t. [4]

Question 2 Derive an ordinary differential equation (ODE) which describes the evolution of the mean number of particles, M, in terms of the moments of A and simplify as far as possible. [4]

Question 3 Apply the mean-field moment closure to the equation in Question 2 in order to derive a closed evolution ODE for the mean. [1]

Code up the stochastic version of the model in Matlab, representing reactions as exponentially distributed events with the appropriate rates. In the case of incorrect answers I may look at your code to try to award marks. All code should be commented to the standards seen in class. I will not attempt to read uncommented code.

Question 4 Plot the evolution of the average (where the average is taken over 1000 independent repeats) numbers of particles against time for the time interval $t \in [0, 100]$. Include the plot in your answer document. [6]

Question 5 Using your code adapted from Question 4, find and state the steady state values of the mean and variance of the number of particles to within ± 0.1. [2]

Question 6 Numerically solve the mean-field ordinary differential equation you derived in Question 3 and plot it on top of the output from Question 4 and include the resulting plot in your answer document. [2]

Question 7 Give the steady state value of the mean number of particles predicted by the mean-field equation in Question 3. [1]

Question 8 Use the master equation to derive an equation for the evolution of the second moment of the numbers of particles. [6]

Question 9 Close the equation derived in Question 8 using the normal moment closure. [2]

Question 10 Solve numerically the closed system of ODEs derived in Questions 2 (for the mean) and 9 (for the second moment) and comment on the steady state values for the mean and variance compared to those found in Question 5 for the full stochastic simulation. [5]

Question 11 Plot the stationary probability distribution of system (1), as found by long run stochastic simulation, as a histogram. Ensure you have done enough repeats of the stochastic simulation to ensure the bars of the histogram vary smoothly. Plot the normal distribution (with mean and variance found computationally in Question 5) as a red curve on top of the histogram. Include the figure in your answers document. Comment on the quality of the agreement of the two distributions with reference to the agreement between your answers in Questions 5 and 10. [5]

Question 12 Code up a $\tau-$leaping simulation of reaction system (1). Calculate the mean value of the solution at steady state averaged over at least 1000 repeats of the $\tau-$leaping simulation. Plot the absolute value of the difference between the mean steady state value predicted by the $\tau-$leaping simulation and the mean steady state value found in Question 5 for $\tau = 1, 0.5, 0.25, 0.125$. Include the plot in your answer document.

Note: If you find that species numbers are becoming negative in some simulations (as is possible with τ-leaping, as mentioned in the long version of the lecture notes), you should mitigate this by setting the negative species to 0 and continuing the simulation. [6]

Question 13 Instead of fixing a time-step and simulating the number of firings of each reaction that occurs during the time-step between updates of the propensity functions as Poisson distributed random variables, consider fixing a number of reactions to occur between updates and simulating an appropriate time-step. This is known as $R-$leaping, where R is the number of reactions to be fired between updates.

Derive the probability density function of the distribution from which the time increment should be drawn.

For a general reaction system comprising M reactions with propensity functions $\alpha_1, \alpha_2 \ldots, \alpha_M$, suggest a scheme for sampling how many of each reaction type should be drawn in order to make up the total of R reactions that fire between updates. [6]

Submission: Electronic answers (typed report or hand-written and scanned) and code (5 `.m` files max - you do not need to submit exportfig.m if you use this) should be submitted electronically via moodle by 12 noon on Friday 8th December 2023. Please title your document in the following format:

`{candidate_number}_{2023}` and ensure your candidate number is appended to the title of your code(s).

Please ensure your answer document is submitted as a PDF.